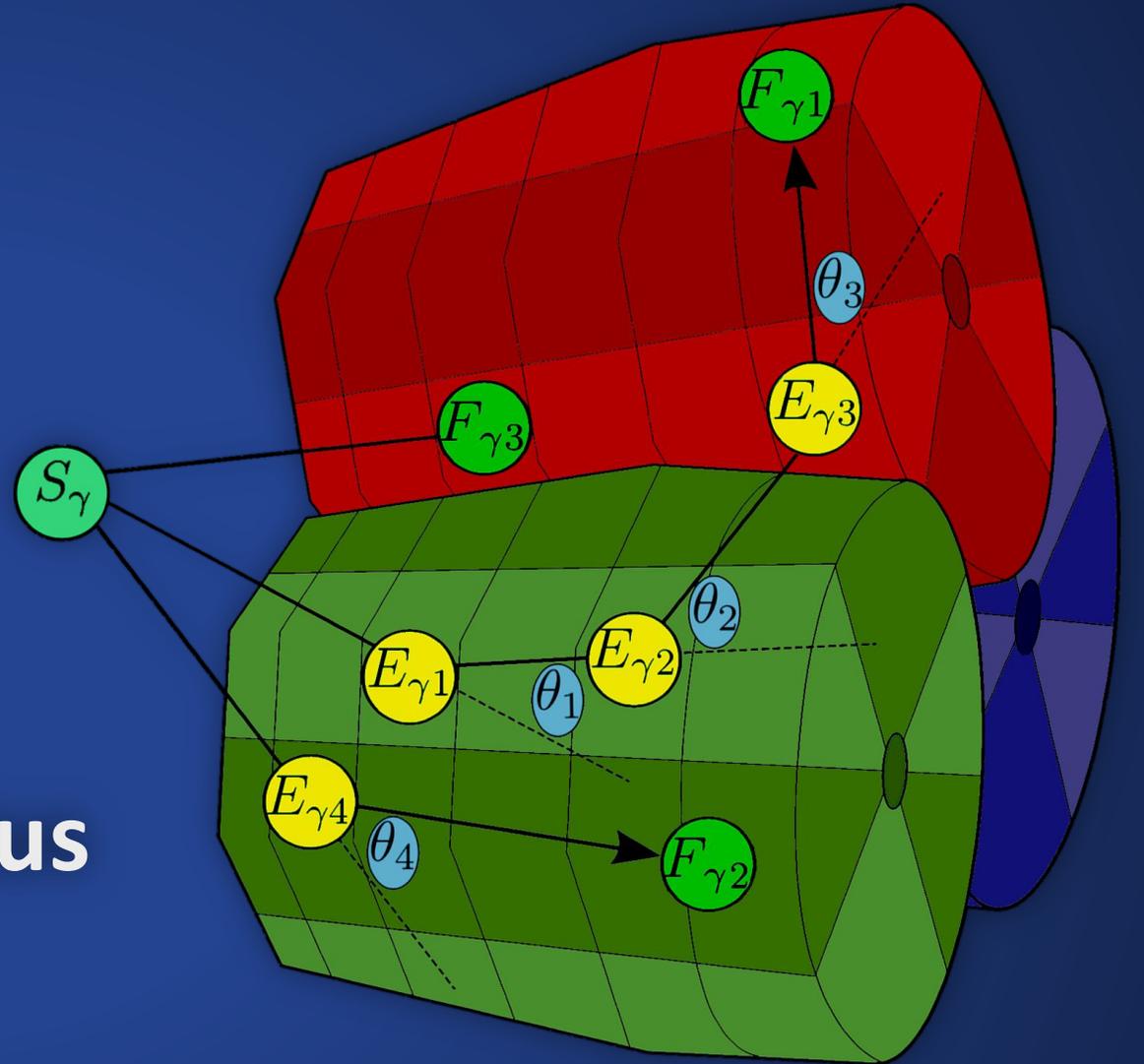


Liverpool R&D: (ML/AI) Status

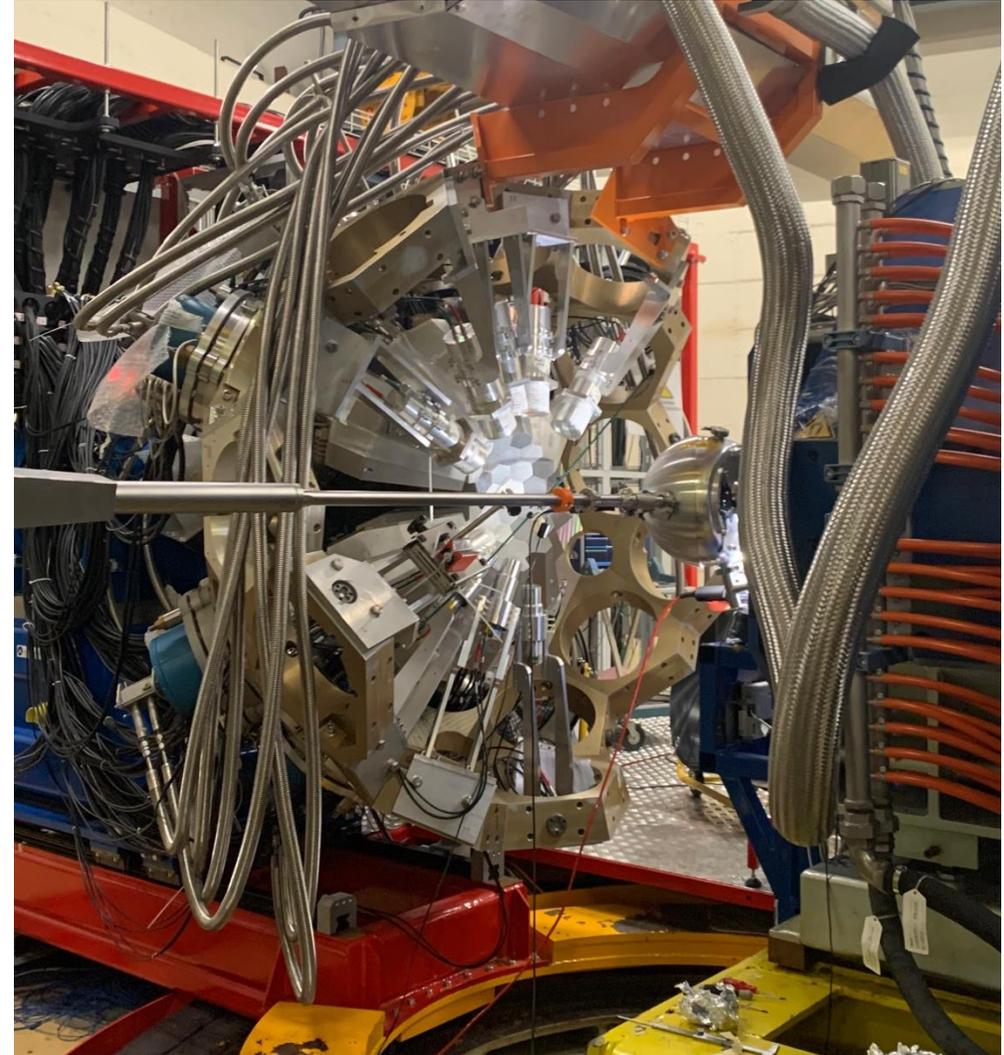
Dr. Fraser Holloway

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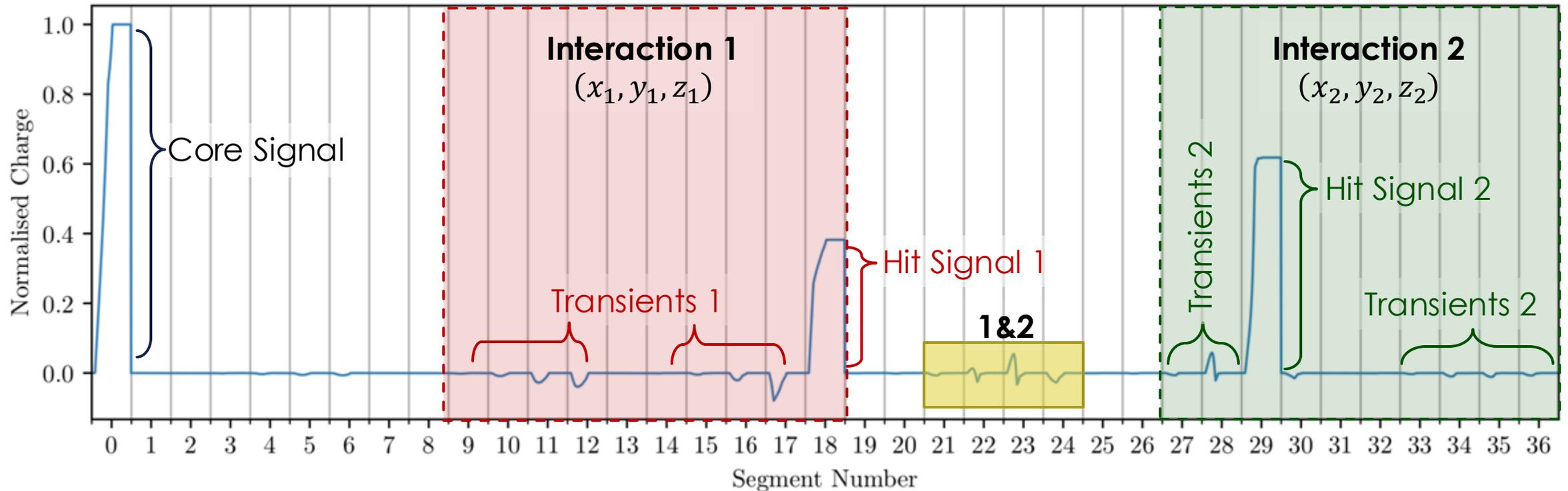
- ▶ AGATA signal response
- ▶ Parametric vs Optimisation based PSA
- ▶ Recap of SIMPLEX PSA algorithm
- ▶ Initial results & issues
- ▶ Masking within AGAPRO
- ▶ Dual-Segment PSA
- ▶ Crystal-wide Optimisation
- ▶ Intelligent Preprocessing



AGATA at LNL (22/10/23)

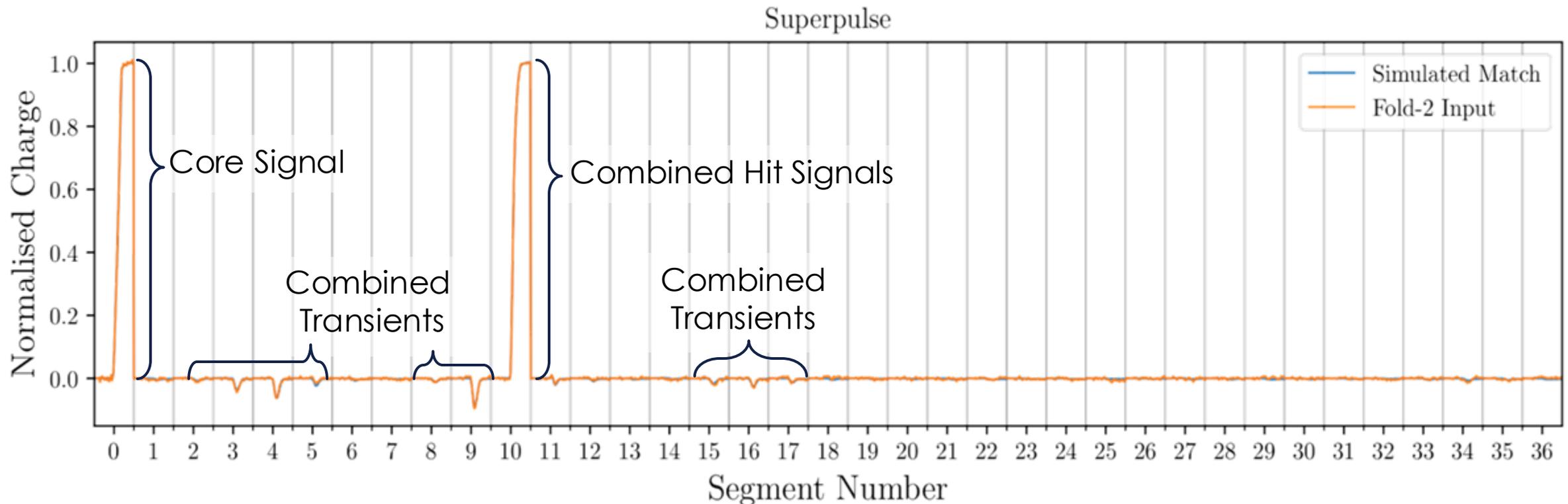


- ▶ High-Fold signals are separated and processed individually when possible.
- ▶ Conventionally this is achieved using segment windows, renormalisation & recursive subtraction.
- ▶ This only works on well-separable signals, typically a few segments apart.





- ▶ These can look near-identical to Fold-1 signals and will regularly fool parametric, PSA & ML methods.
- ▶ The underlying signals are heavily entangled and cannot be solved individually.
- ▶ They have massive implications for tracking (e.g. a $[60^\circ, 30^\circ]$ scatter pair looking like a 90° scatter).





Within AGATA Pulse Shape Analysis is used to quickly compare experimental signals (M) against simulated signals (S) using a Figure of Merit (FoM).

$$FoM = \sum_{i=1}^{37} \left(\sum_{j=1}^{121} (|M(j)_i - S(j)_i|)^2 \right)$$

The position of the closest match in the basis is then used for the predicted interaction position and given to the GRT.

Current PSA utilises a 2-part grid search (AGS), initial optimisation of a coarse grid followed by a fine-grid search around the local optima.

This work focusses on solving 2-interactions within the same segment for AGATA.

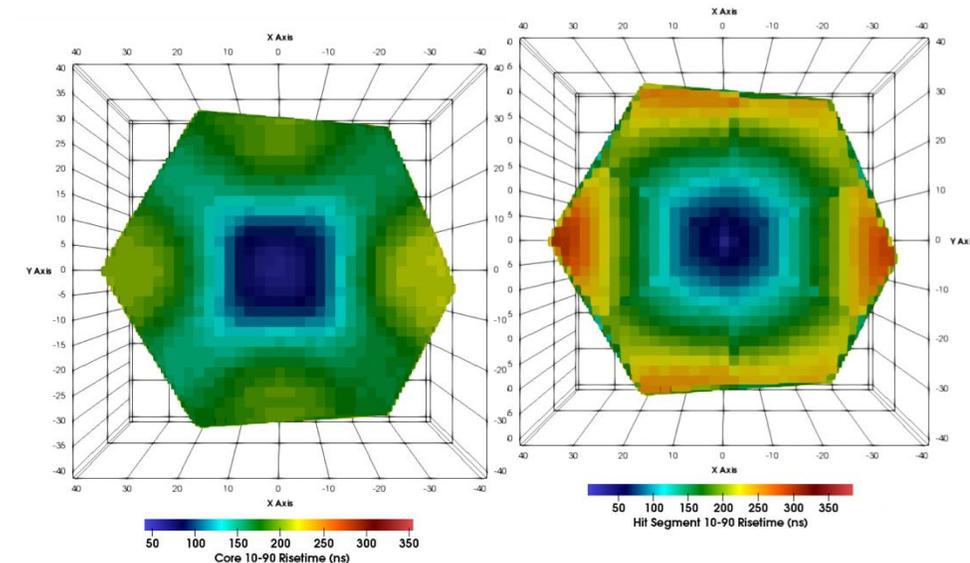
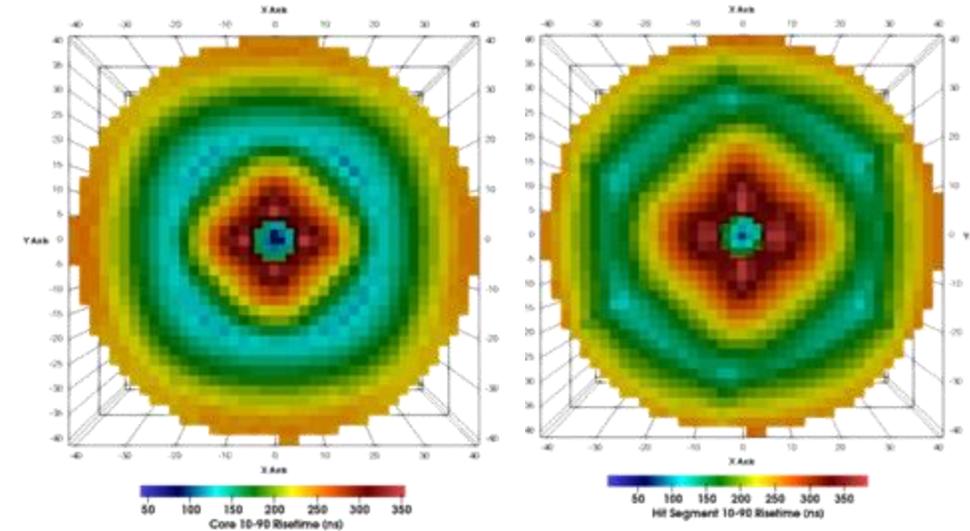


Parametric PSA concerns features that can be easily derived (T_{10-90} , ICA)

- ▶ These methods are easy to program, simple to apply to ASICs & FPGAs
- ▶ They are typically surjective (many positions have the same value).
 - ▶ Insufficient for use in γ -ray localisation & tracking.
- ▶ Apply poorly to multi-interaction PSA.

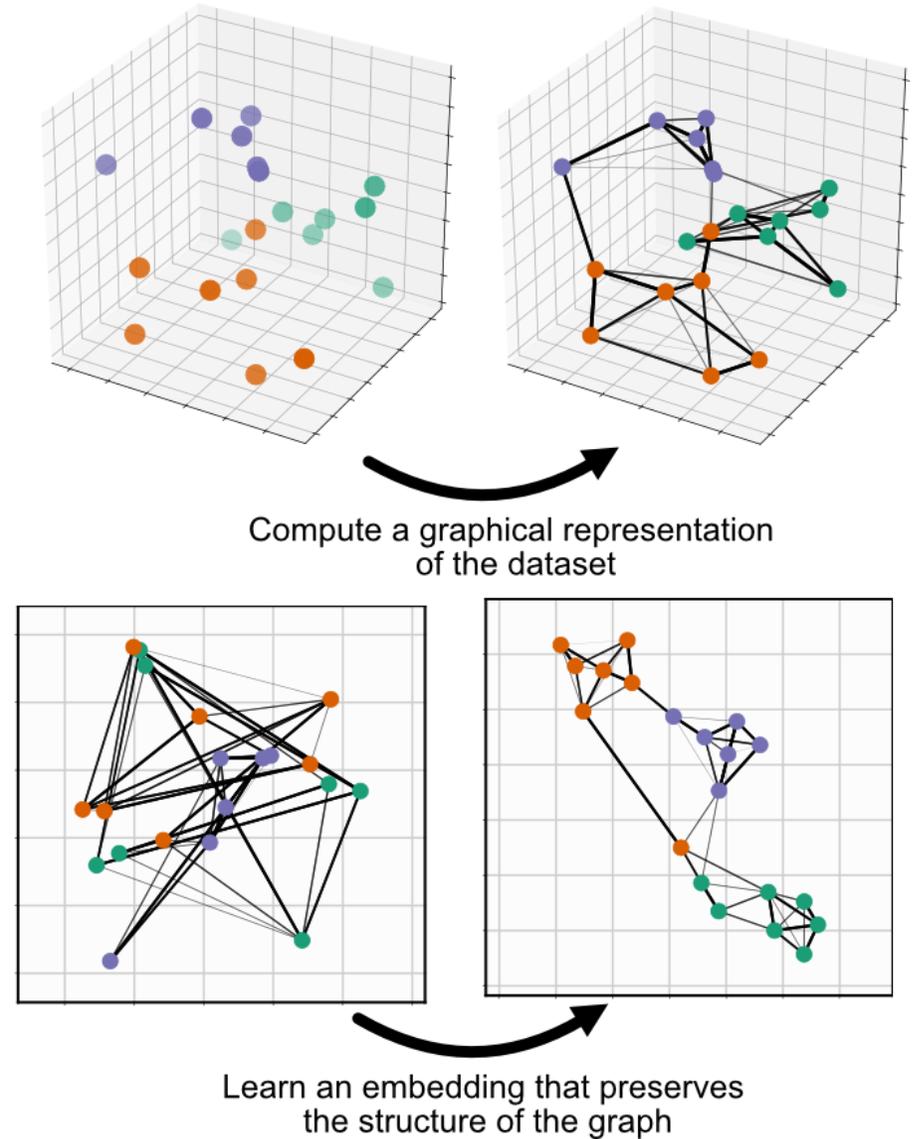
Non-parametric PSA concerns features that are more complex:

- ▶ Components of the signal (e.g. from PCA/SVD or AI)
- ▶ Can be used to form regression predictors (e.g. in CZT)
 - ▶ Inaccurate but fast.
- ▶ Often used in optimisation (k NN) for localisation:
 - ▶ Accurate but slow.



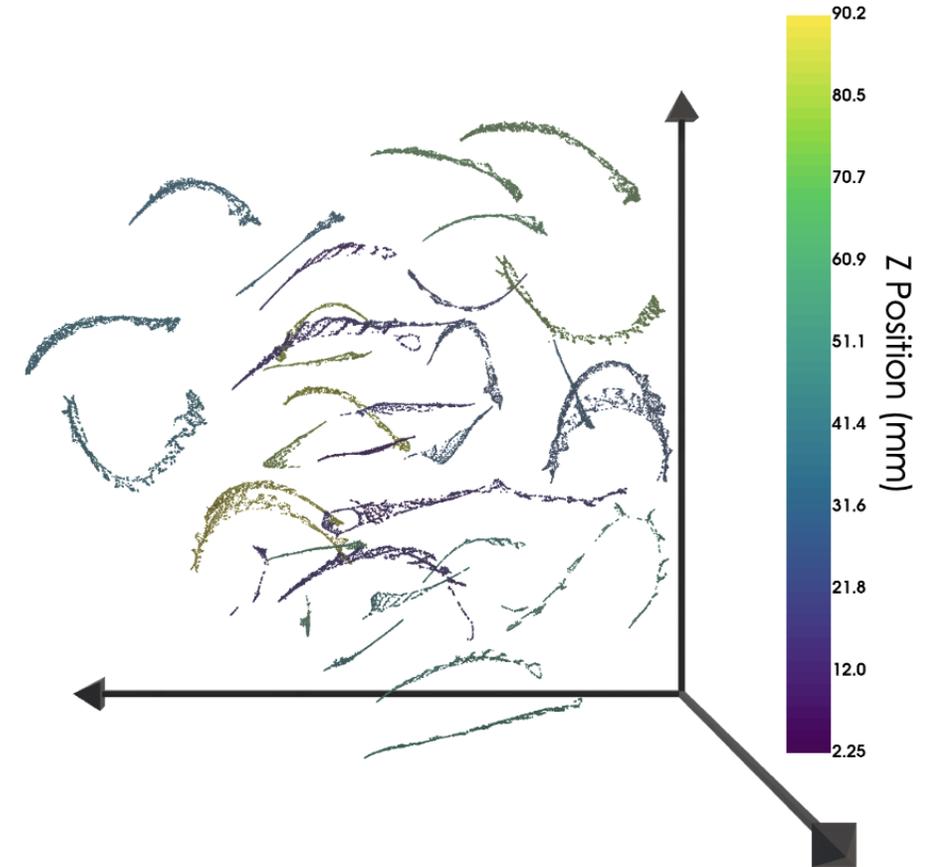


- ▶ Monolithic Coaxial detectors show some signal variation with position, most signals form a continuous response manifold in \mathcal{R}_n .
- ▶ This can be observed with covariance matrices.
- ▶ Alternatively, we can use manifold learning.





- ▶ Segmentation within AGATA provides a wealth of information within the signal response.
- ▶ Detector response goes from temporal to spatiotemporal.
- ▶ Segment responses concentrate in submanifolds.
- ▶ Strong radial and azimuthal dependence observed.
- ▶ Transient signals provide additional fidelity (x, y, z).
- ▶ These effects allow for ~ 3 interaction PSA within a segment.
 - ▶ Upper limit of ~ 9 interactions across a crystal.





As part of my work I investigated the use of graph structures to accelerate PSA, they have several marked benefits:

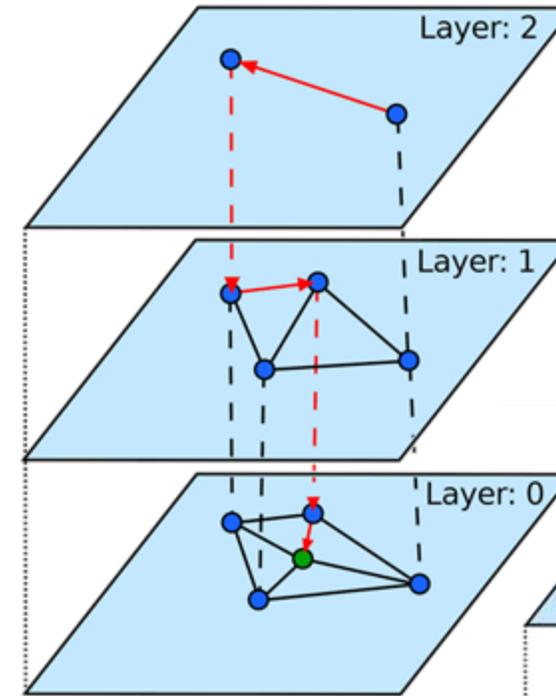
- ▶ Data-driven \therefore no parametric methods (e.g. T_{90}) needed.
- ▶ Self-organised \therefore no rigid grid structure required.
- ▶ Hierarchical \therefore adaptive resolution.

In my work I profiled several methods for accelerated PSA:

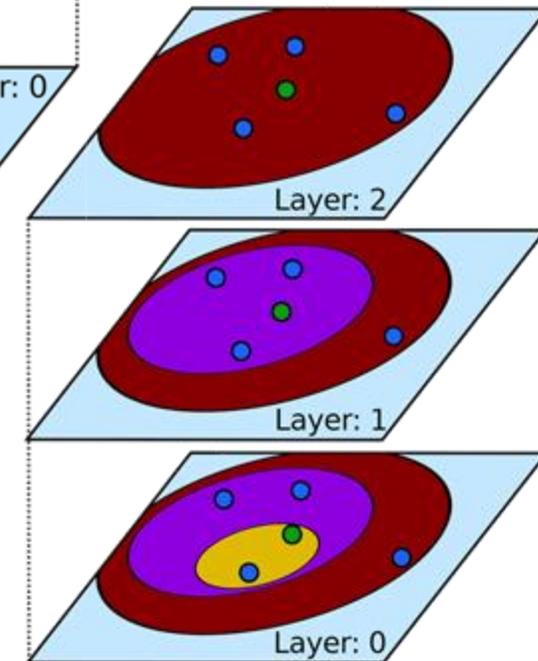
- ▶ Space Partitioning (exact k NN): k D-Tree, M -Trees, etc.
- ▶ Coarse Indexing (approximate k NN): HNSWLib, FAISS.

Recommendations from this work are being implemented.

- ▶ My current work is focussed on multiple-interactions.



HNSW Structure



M-Tree Structure



Multiple interaction events make up a significant fraction of the data collected by AGATA.

Around 30% of events in AGATA are comprised of events where multiple interactions occur in the same segment.

- ▶ This will vary as a function of γ -ray energy

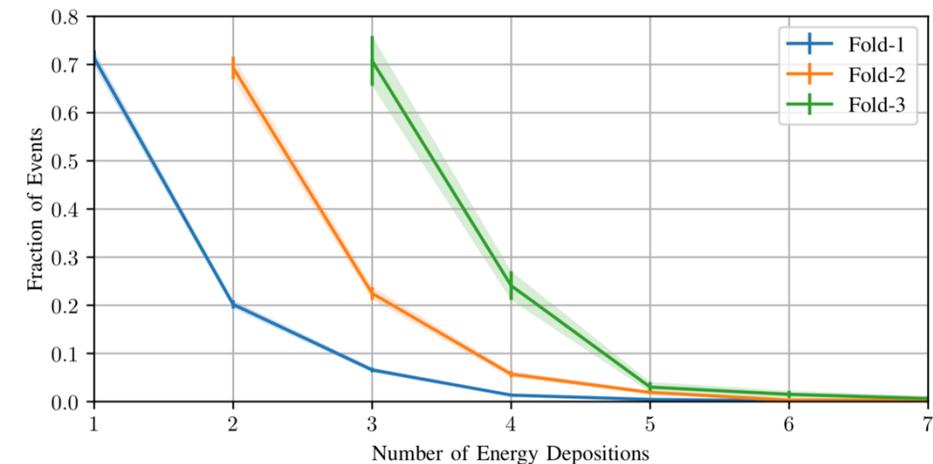
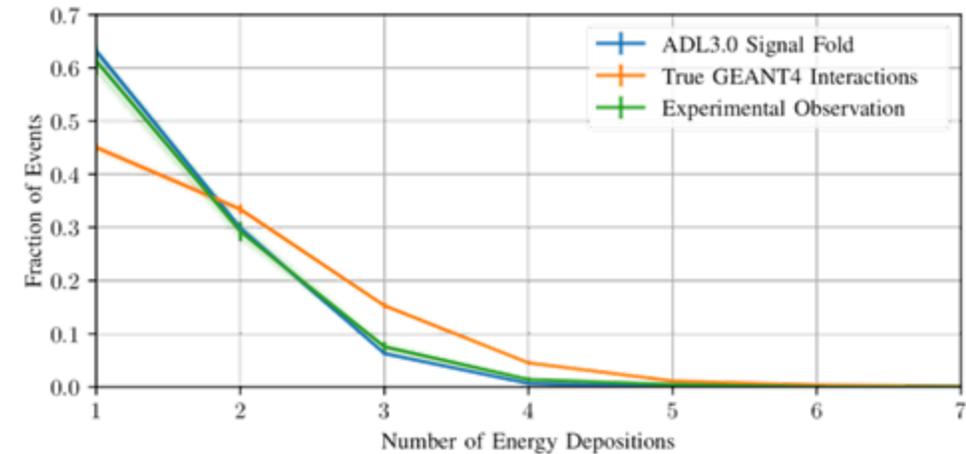
In these cases, the PSA tends to fit a weighted average of the positions.

- ▶ Preference to predict barycentre at segment centres.

Evaluation of multi-interaction events using conventional PSA is not feasible.

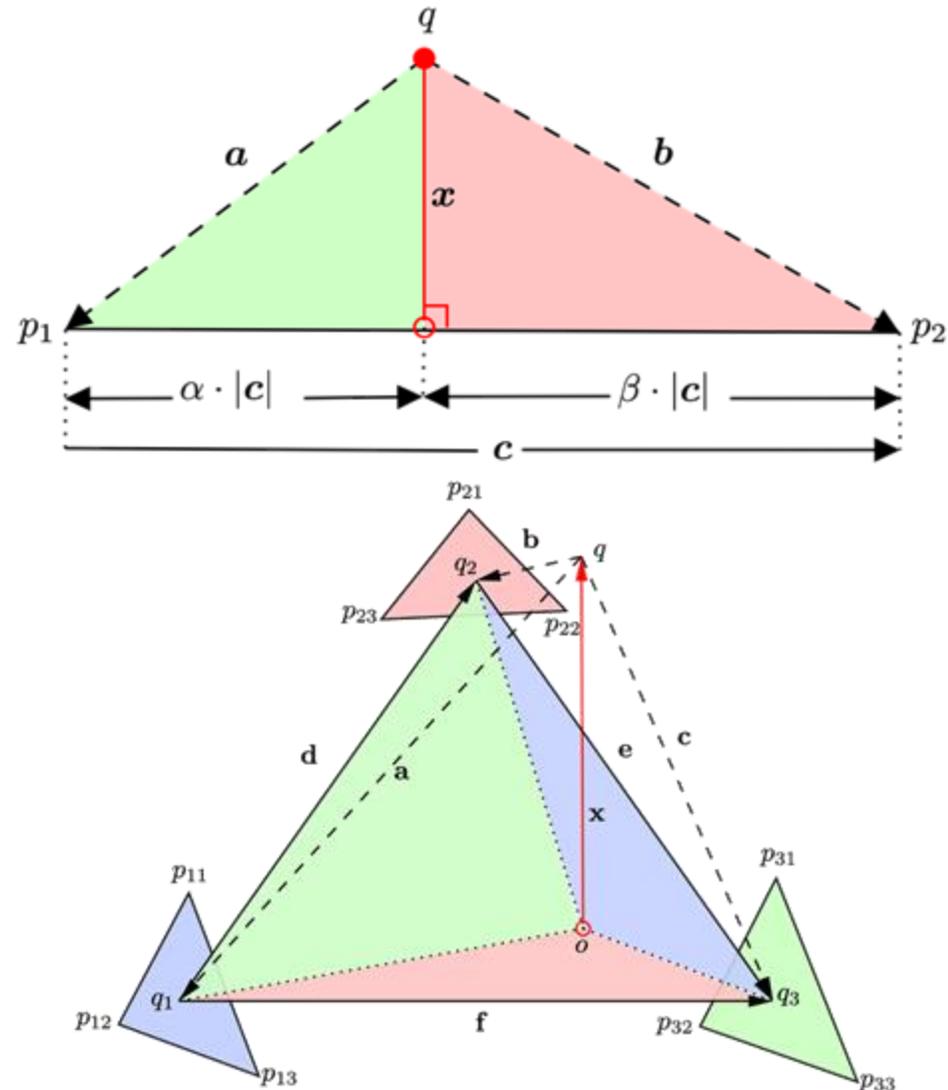
Initial implementation of GRETA algorithm was performed but a flaw was found in their approach that is currently irreconcilable.

- ▶ Currently working with the GRETA team to see if it's fixable.



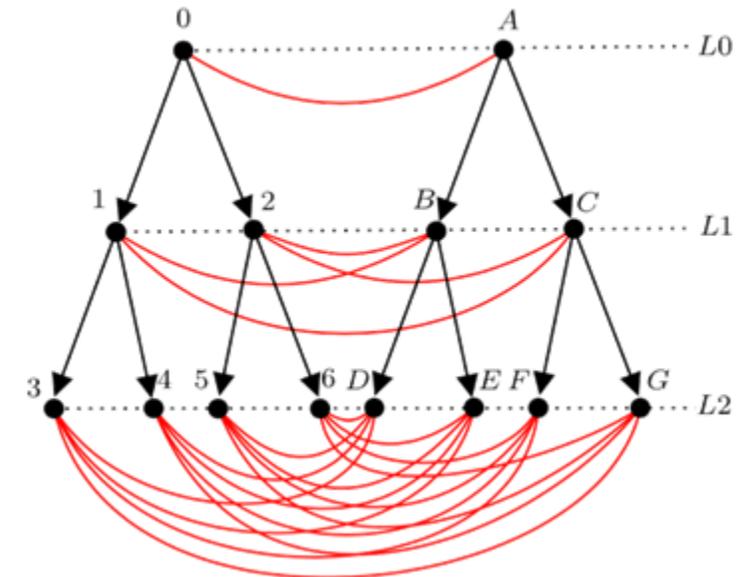
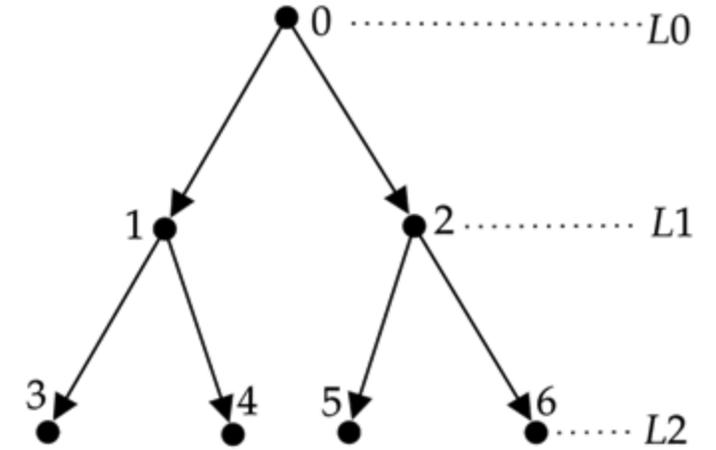


- ▶ A new convention was developed to evaluate multi-interaction signals using distance geometry and simplex de-mixing.
 - ▶ $\overrightarrow{Op_1} \cdot \overrightarrow{qO} = \overrightarrow{Op_2} \cdot \overrightarrow{qO} = \overrightarrow{p_1p_2} \cdot \overrightarrow{qO} = 0$
 - ▶ $\angle Op_1p_2$ & $\angle Op_2p_1 < 90^\circ$
- ▶ This convention allows for direct fitting of multi-interaction signals.
 - ▶ Also works recursively, allowing for 9-interaction fits.
- ▶ Exhaustive combinations are required to find the best solution:
 - ▶ ~1,100,000 combinations for 2 interactions.
 - ▶ ~550,000,000 combinations for 3 interactions.
 - ▶ $\sim 10^{30}$ combinations for 9 interactions.
- ▶ Not feasible to do on a CPU exhaustively real-time.
 - ▶ Somewhat possible on a GPU.
 - ▶ How about using graph acceleration?





- ▶ 2-interaction solutions exist as edges that connect between nodes of two orthogonal trees.
- ▶ Lower levels have more nodes \therefore more edges.
- ▶ Just like how nodes can have child nodes edges can have child edges.
 - ▶ The validity of an edge applies recursively.
 - ▶ If an edge is invalid, all child edges are also invalid.
- ▶ This allows for us to cull large sections of the graph.



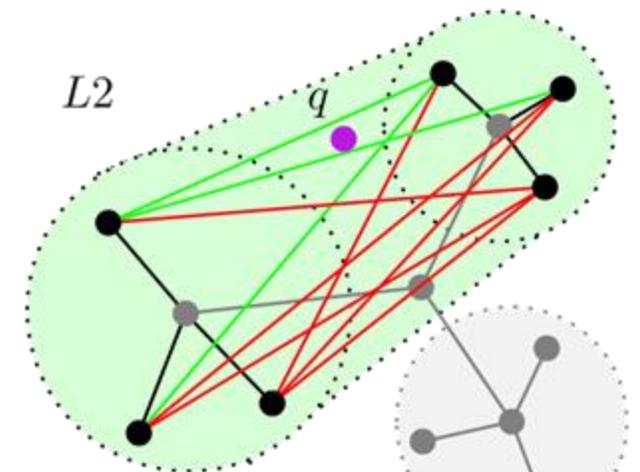
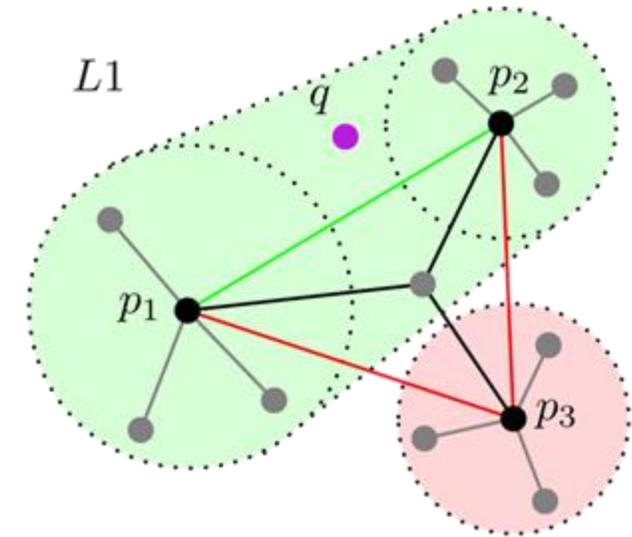


Two hypergraph-accelerated methods have been developed:

- ▶ Hyper- M -Tree
 - ▶ Recursive covering (Exact k NS search).
- ▶ Hyper-Hierarchical New Small World Graphs.
 - ▶ Greedy simplex traversal (Approximate k NS search).

These overcome conventional limitations of the existing method:

- ▶ Native support for PSA uncertainty
- ▶ Self-learned hierarchy.
- ▶ Support for dynamic resolution (FEM) bases.



Coverage pruning



SIMPLEX and GRETINA PSA codes have been implemented within AGAPRO;

- ▶ Exhaustive & AGS approaches available.
- ▶ Rudimentary support for uncertainty propagation.
- ▶ Accelerated using SIMD instructions.

A flaw was found in the precomputation step W.R.T masking of distances

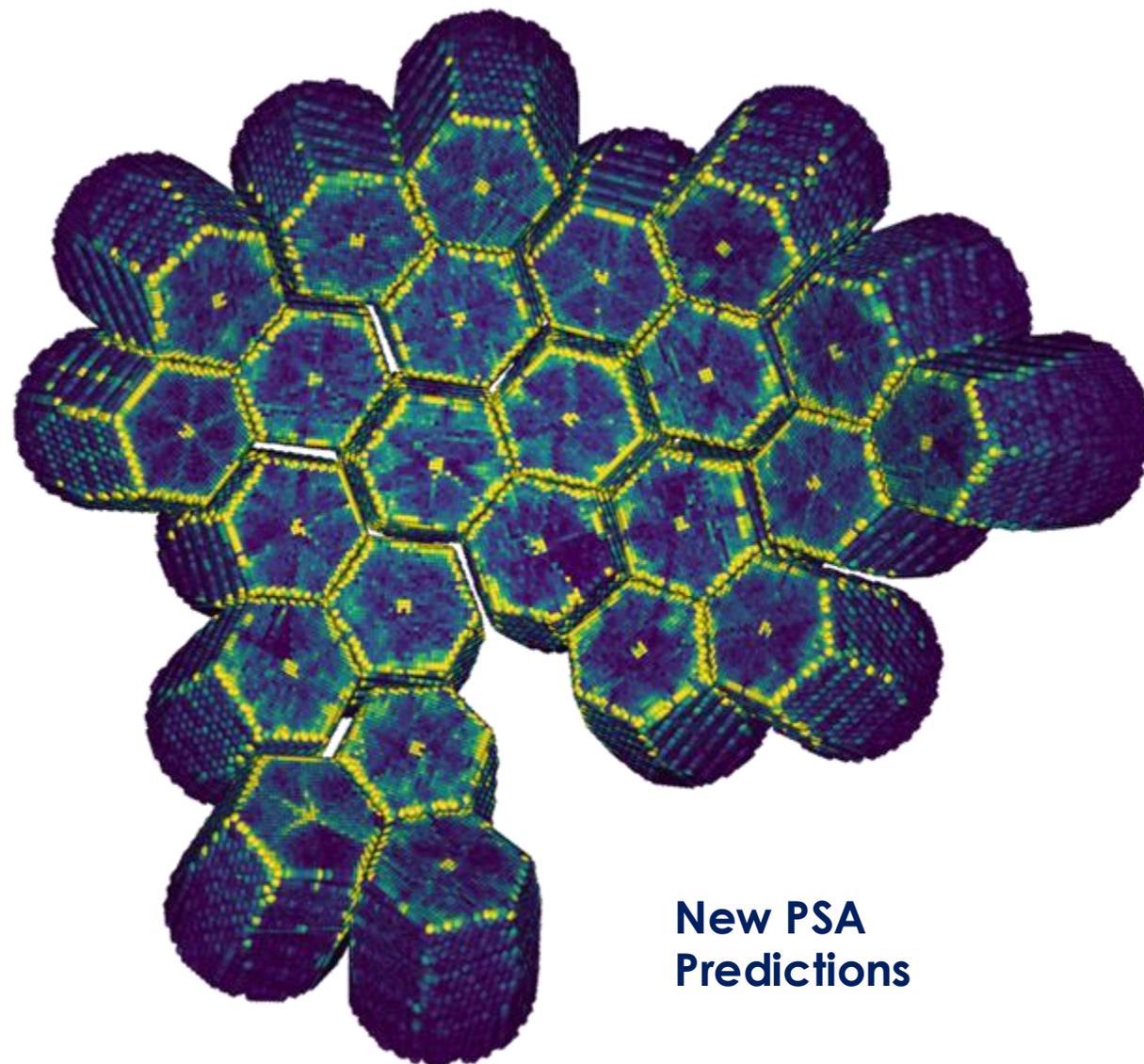
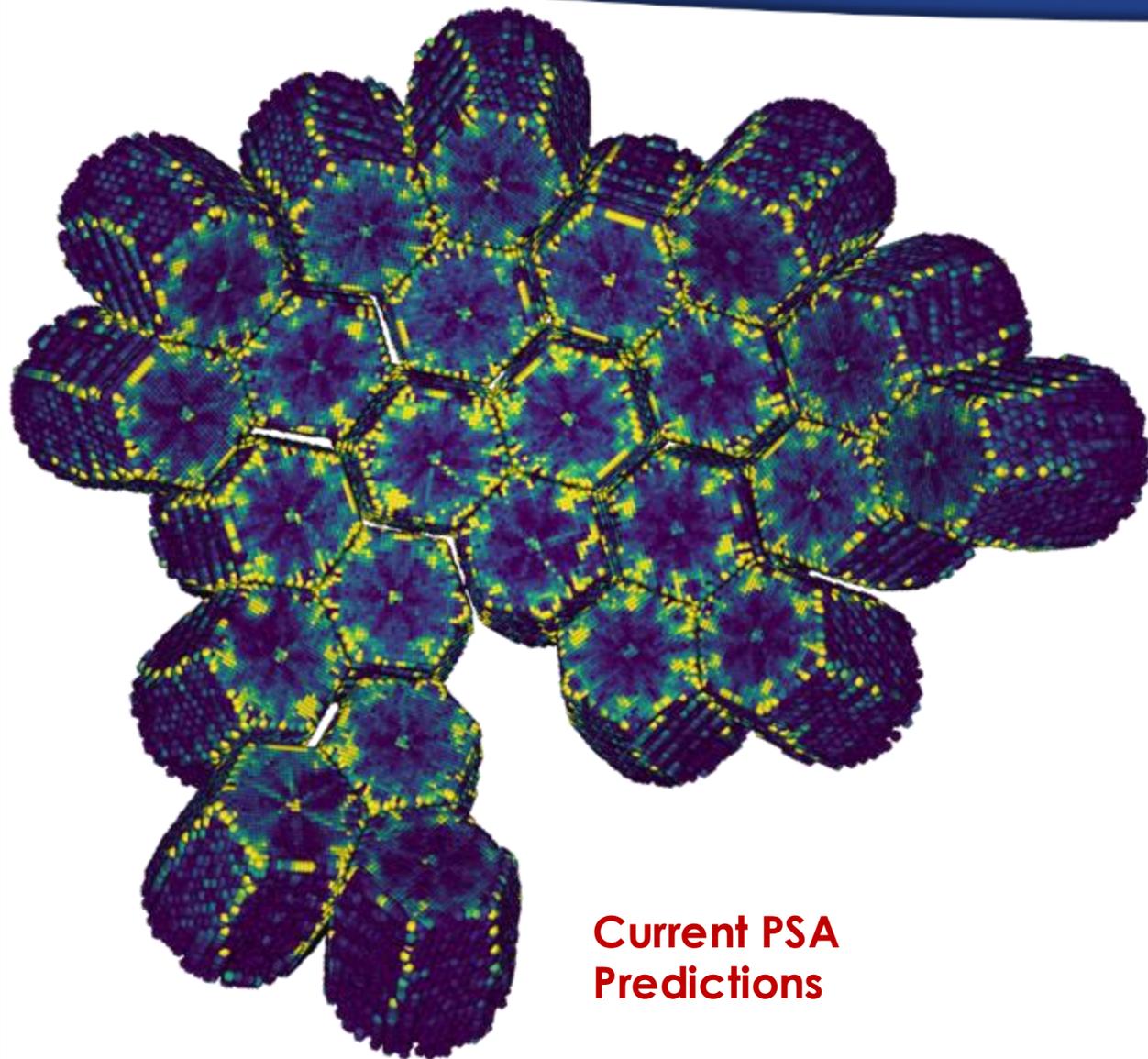
- ▶ Investigating the remedy uncovered other issues unrelated to the new algorithm.
- ▶ Currently working on a more comprehensive PSA pipeline.
 - ▶ Better handling of single vs multi-interaction events & Recursive Subtraction & Time-shifting.
 - ▶ Integrates a more intelligent preprocessing using ML.
 - ▶ Will have a crystal-wide optimiser for the full superpulse.

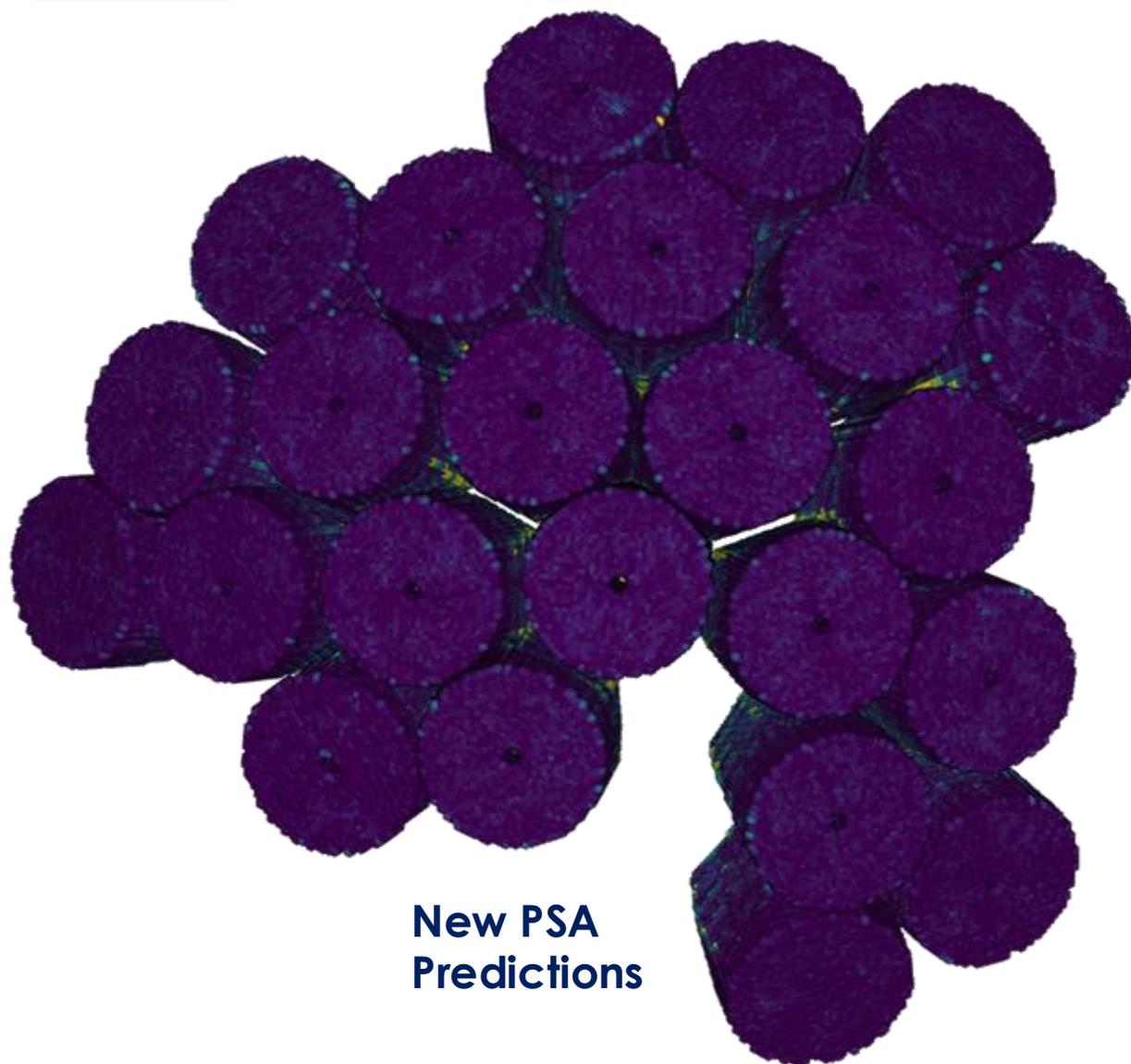


- ▶ A dataset was extracted from E680 at GANIL, fission ^{98}Zr nucleus with a strong γ -ray transition at 1.2 MeV.
- ▶ Fragments were emitted with velocities of $\beta \approx 10$, making the resolution of such transition strongly dependant on the quality of the Doppler correction.
 - ▶ Doppler correction only applies to first interaction.
- ▶ PSA also will heavily influence tracking accuracy.
 - ▶ Should influence peak prominence.

Important note:

- ▶ The spectral performance of AGATA is the combined effect of PSA, GRT & simulated bases accuracy.
 - ▶ GRT has yet to be tuned for the new PSA.
 - ▶ Bases are being recalculated at higher fidelity.
 - ▶ **This is all with the current flaws, I am working on fixes.**
 - ▶ **Performance will likely change in the future.**





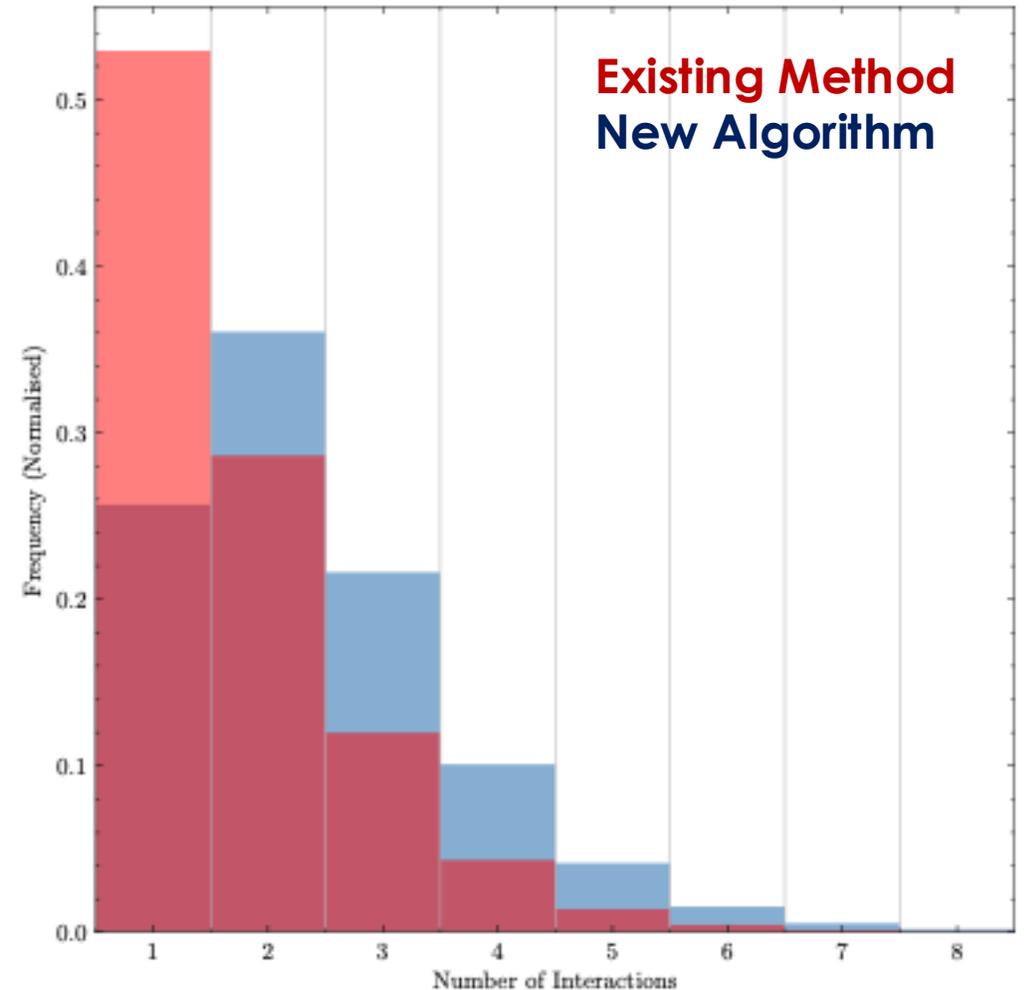


Observed number of interactions changes drastically with the new algorithm

Prevalence of single-interaction signals is reduced significantly, average track length increased.

Previously 44% of tracks were P.E single-site

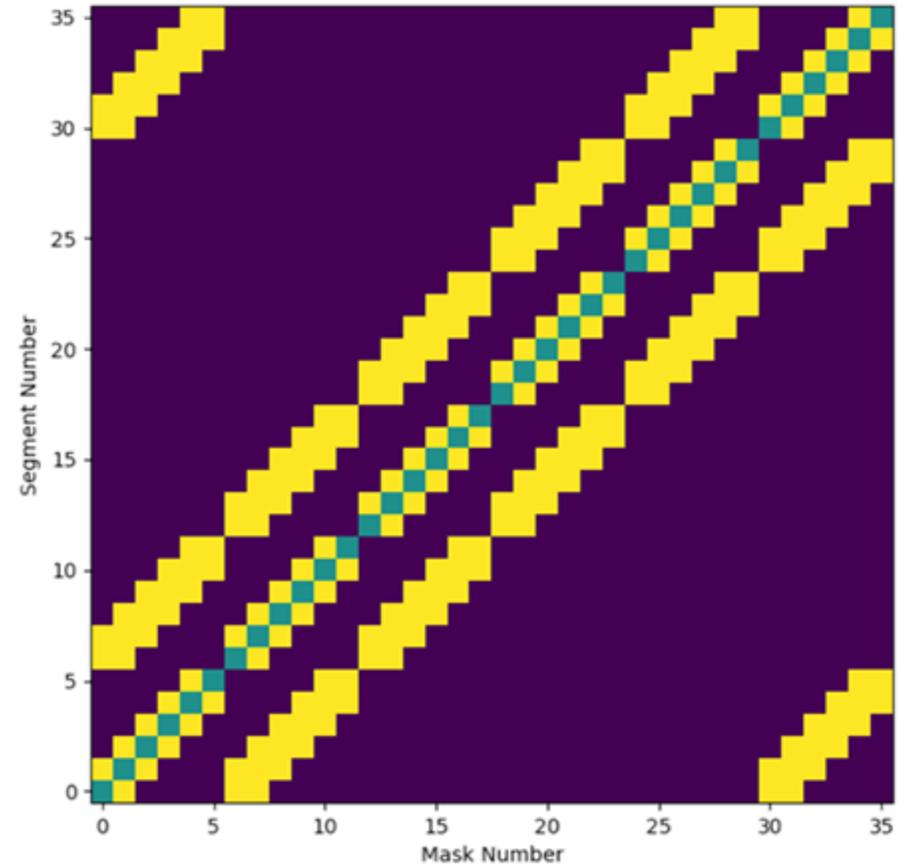
Now only 17% are P.E single-site





Whenever a signal is processed in AGAPRO a window is created to allow PSA to process events independently.

- ▶ This occurs roughly 2/3 of the time.
- ▶ Comes in two forms `hmask` & `lmask` (& `nmask`):
 - ▶ `hmask` is pre-event, depends on the hit segment.
 - ▶ `neighbours = -2`
 - ▶ 36 static masks that are well-known.
 - ▶ `lmask` is live, depends on the other events in the crystal.
 - ▶ Removes other net charge signals.
 - ▶ Could remove neighbour transients, currently disabled.
 - ▶ Around 3500 unique masks
- ▶ Because `lmask` changes for each event the precomputed distances are directly affected.
 - ▶ This is problematic, there are 35 million of them.

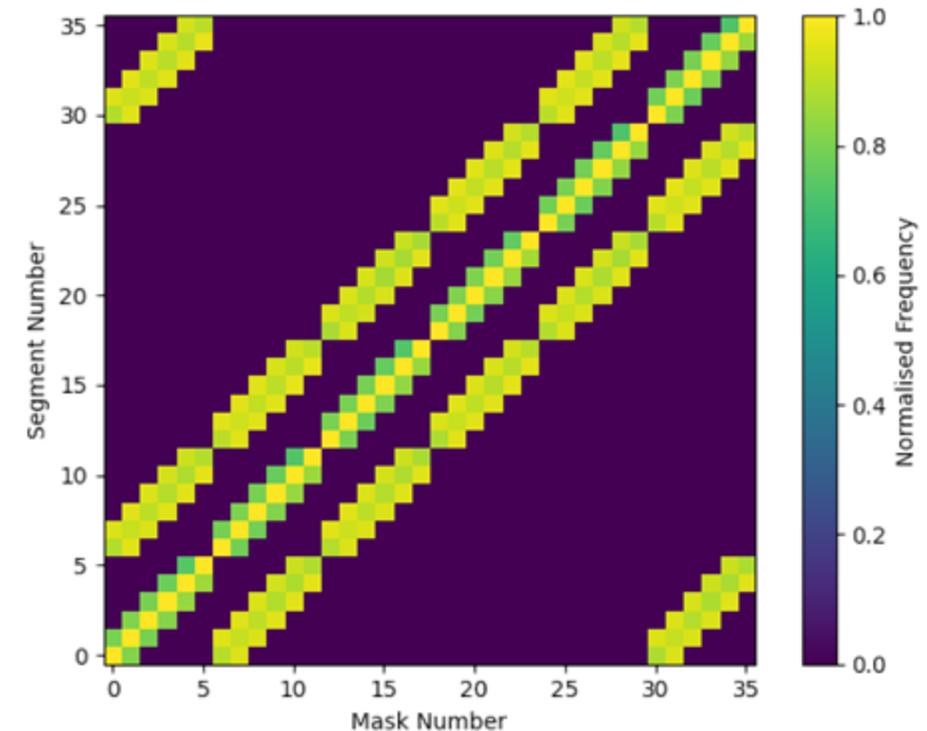


Observed hmask



Whenever a signal is processed in AGAPRO a window is created to allow PSA to process events independently.

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 - ▶ This is problematic, there are 35 million of them.



`lmask` Frequency (normalised)



Precomputed distances are a key part of the multi-interaction algorithms, vastly outnumber novel distances.

- ▶ Segment 6 has ~2,000 novel distances, ~2,000,000 precomputed.
- ▶ Distance computation is expensive, 1-2,000 float operations each time.
- ▶ Having to re-compute d_c for each event is not feasible to do real-time.

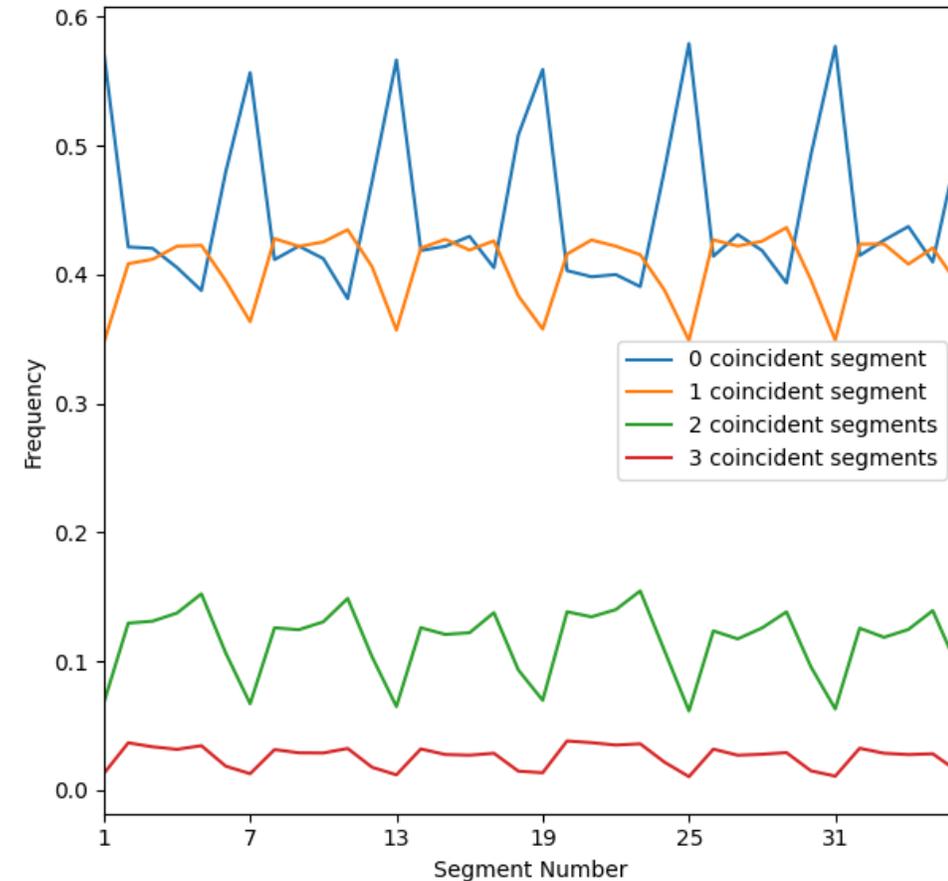
Thankfully $L2^2$ is commutative, can be split into sub-distances:

- ▶ d_c can be precomputed for each segment, summed once the `lmask` is determined
 - ▶ Requires significant memory increase of ~36x
- ▶ Could be optimised using Boolean Covering to find prime implicants using Quine-McCluskey algorithm.
- ▶ d_c can be precomputed for `hmask` and its components
 - ▶ Calculate `hmask` distance and then subtract `lmask` components
 - ▶ Slightly better memory efficiency, only 8x previous version
- ▶ Current RAM utilisation is 6 GB/crystal, could be reduced to ~2.5 GB



Occurrence of hits that influence l_{mask} is around 63%, vast majority occur in neighbouring segments.

- ▶ Even without removing neighbours of coincident events the l_{mask} is significantly reduced.
 - ▶ Some PSA is run on a single segment, not great.
 - ▶ Presence of transients is not accounted for, will affect PSA.
 - ▶ Removing the neighbour segments altogether is worse.
- ▶ 2-interaction PSA is not explicitly limited to a single segment.
 - ▶ Can be modified to run on the full crystal.
 - ▶ Significant memory requirements again, ~32x larger
 - ▶ Can be modified to run on overlapping windows.
 - ▶ Slightly better, 8-12x larger.





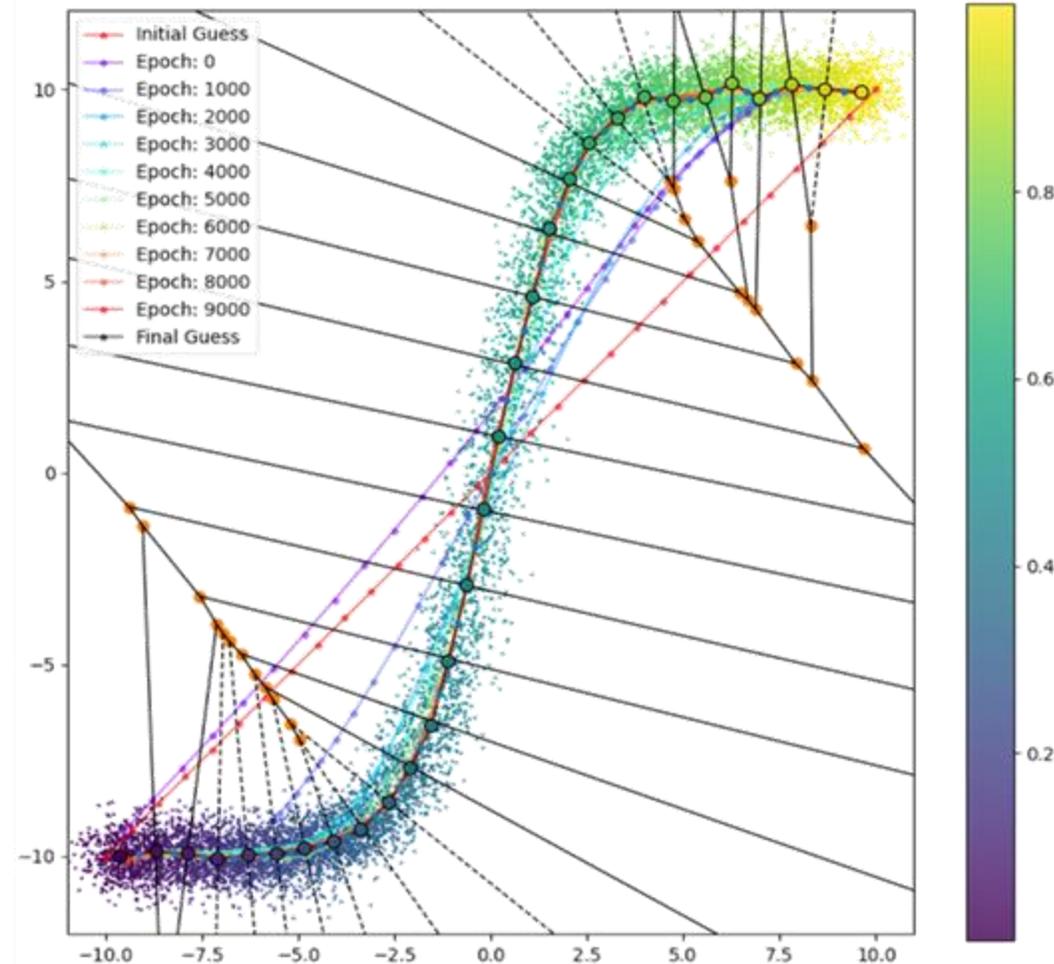
- ▶ Within AGAPRO PSA the superpulse is separated into windows, and processed at the segment level.
 - ▶ Masking minimises contributions from other interactions but is not perfect.
 - ▶ No way to account for transients on net charge signal.
 - ▶ Fitting errors affect subsequent fits.
 - ▶ A global fit across multiple clusters isn't feasible.
 - ▶ Mathematically possible, but time and memory consuming.
- ▶ Formalism for a generalised solution for n -interactions was developed.
- ▶ This allows for a crystal-wide solution to be found for the full superpulse, not just each window.
- ▶ The best 1 & 2 interaction solutions for each segment can be passed to a global fitter.
 - ▶ A global solution is then found from the reduced set.
 - ▶ Allows for crystal-wide re-optimisation of energies, even within the same segment.



- ▶ 2-interaction PSA is a time-consuming process.
- ▶ Assessment of 1 vs 2 interactions is performed after PSA search via fallback vetoes:
 - ▶ Interaction separation.
 - ▶ Energy fraction & absolute energy.
 - ▶ χ^2 reduction.
- ▶ It'd be useful to skip the 2-interaction PSA if it's unlikely to give a good result.
- ▶ Can we infer what the expected χ^2 , energy fractions & separation are before PSA?
 - ▶ If so, then can we only run 2-interaction on events that will show an improvement?
 - ▶ Can this information provide a better starting guess for PSA?



- ▶ Self-Organising Maps are a graph-ANN that use competitive learning to fit maps to an underlying manifold of data.
- ▶ The map is initialised and slowly iterates to form a topologically constrained approximation of the data.
- ▶ Nodes in the graph then learn from their immediate surroundings via inference.
- ▶ Often used for clustering and feature detection.
- ▶ I've adapted them for polylinear regression.



SOMs for Pseudo-Parametric PSA

25



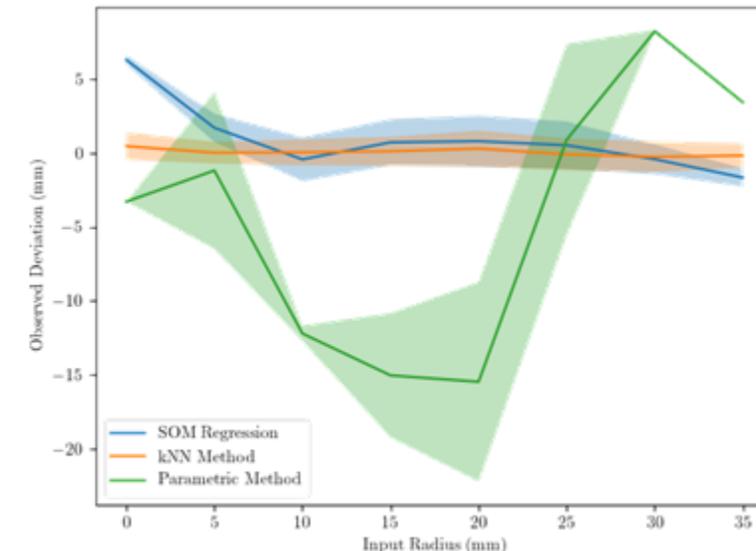
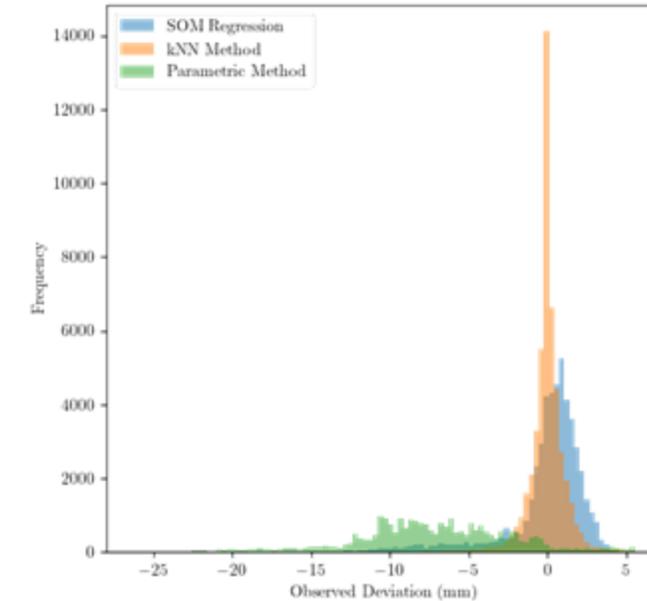
- ▶ SOMs can be augmented with existing analytical PSA techniques to perform regression.
- ▶ Map is converted into a simplicial complex.
- ▶ This allows for a poly-linear segmentation of the response space.
- ▶ Deviations from the map spline can be considered noise.
 - ▶ Significant deviation could be considered multi-interaction.
- ▶ Analytical code is easy to accelerate, map is easily tuneable.
 - ▶ Multithreaded capable of running at 3 MHz.
 - ▶ Can be implemented on FPGAs, Digitisers.
- ▶ Should work for multi-input regression:
 - ▶ Estimate both regression parameters and energy fractions.
 - ▶ Maths is very long, requires 4-interaction PSA.



**AGATA Response
(UMAP Embedding)**

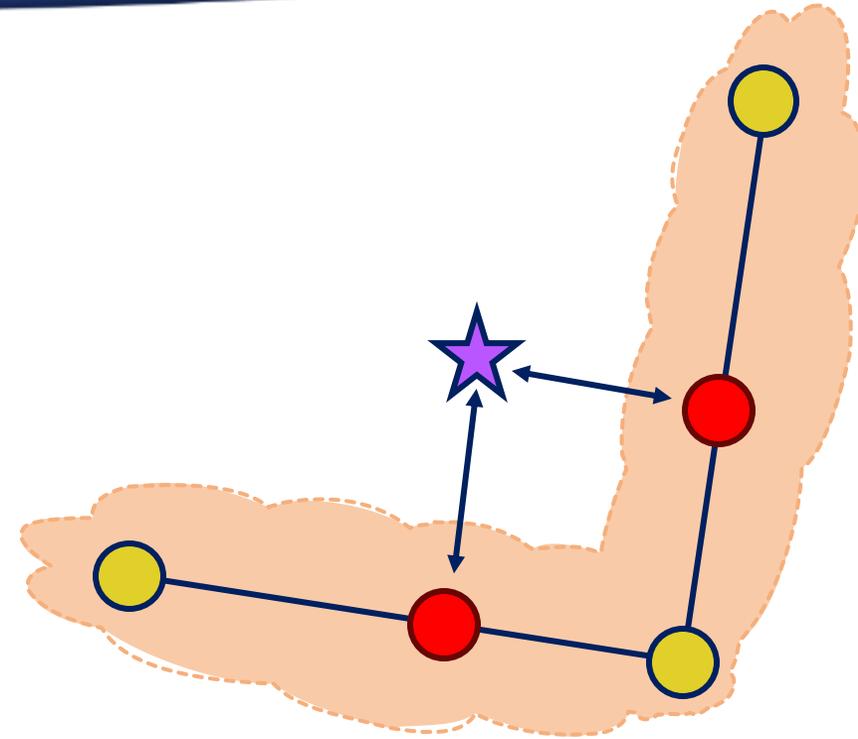


- ▶ SOM was initially trained on simulated AGATA basis (A005).
- ▶ Further refinement using experimental data.
- ▶ Inference then applied to learn radial position.
 - ▶ Should be able to learn t_0 offset & neutron damage.
- ▶ Initial experimental results look promising:
 - ▶ Worse performance than k NN, better than parametric.
 - ▶ Limitations in interpolation, will be fixed with GSOMs.
- ▶ Implementation of FPGA-native code ongoing.





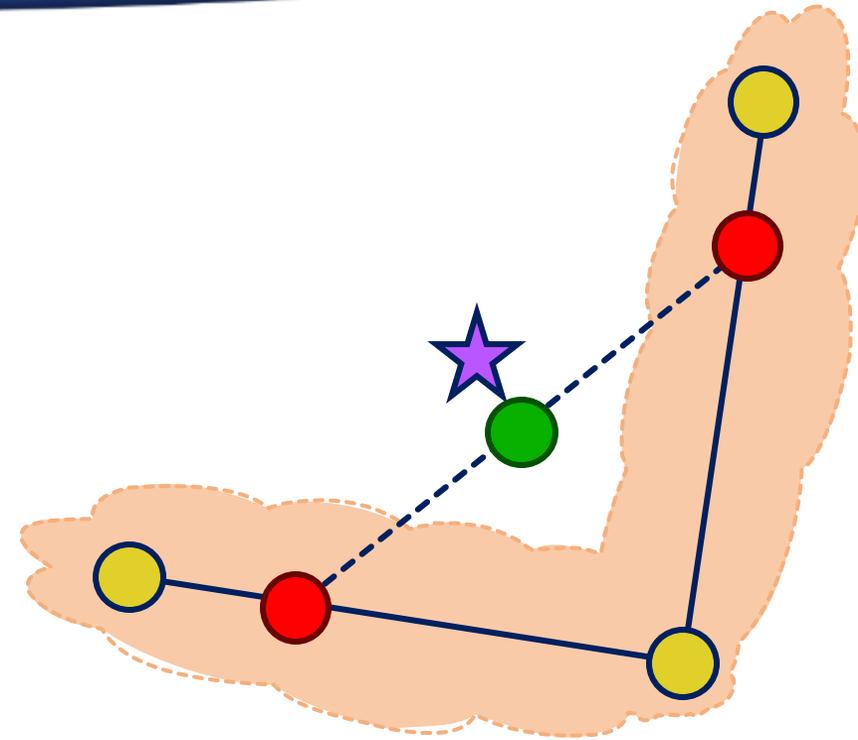
- ▶ The number of interactions can be inferred by estimating the χ^2 for approximations of the underlying manifold.
- ▶ 1-interaction SOM approximation requires determining best simplex interpolation in the map.
 - ▶ Essentially conventional 2-interaction PSA.
- ▶ 2-interaction SOM approximation requires determining the best interpolation of 2 interpolations.
 - ▶ Essentially conventional 4-interaction PSA.
 - ▶ Solving of a 5-simplex, (hyper-hyper tetrahedron).
 - ▶ Moderately difficult.
- ▶ If the χ^2 for the 2-interaction approximation is significantly better we can assume the full search will do the same.
- ▶ If the χ^2 for the 2-interaction approximation fails the vetoes we can assume that the full search will fail to find a good solution either.



Signal Manifold
SOM Nodes
Experimental Query
1-int Approximation
2-int Approximation



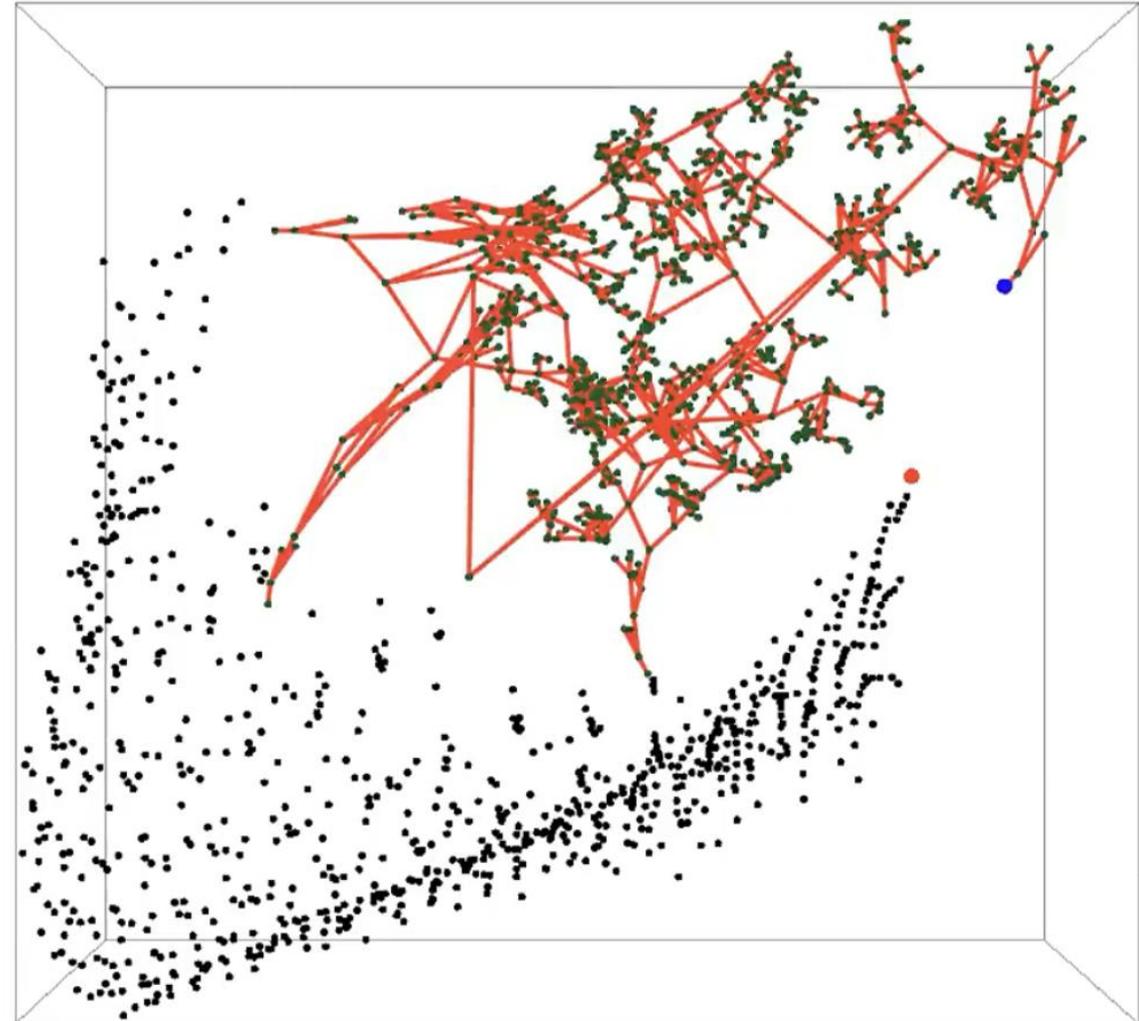
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Signal Manifold
SOM Nodes
Experimental Query
1-int Approximation
2-int Approximation



- ▶ Initial testing of the veto looks promising but needs proper implementation in AGAPRO.
- ▶ Initial predictions of the energy fractions & indices are ignored, could be factored into further PSA.
- ▶ Estimation of t_0 offset would reduce iterative fitting.
- ▶ Ideally should inform predictions of further PSA.
 - ▶ Could be used to build better search structure.



Thanks for Listening

Any Questions?

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Science & Technology
Facilities Council



AGATA
ADVANCED GAMMA
TRACKING ARRAY

