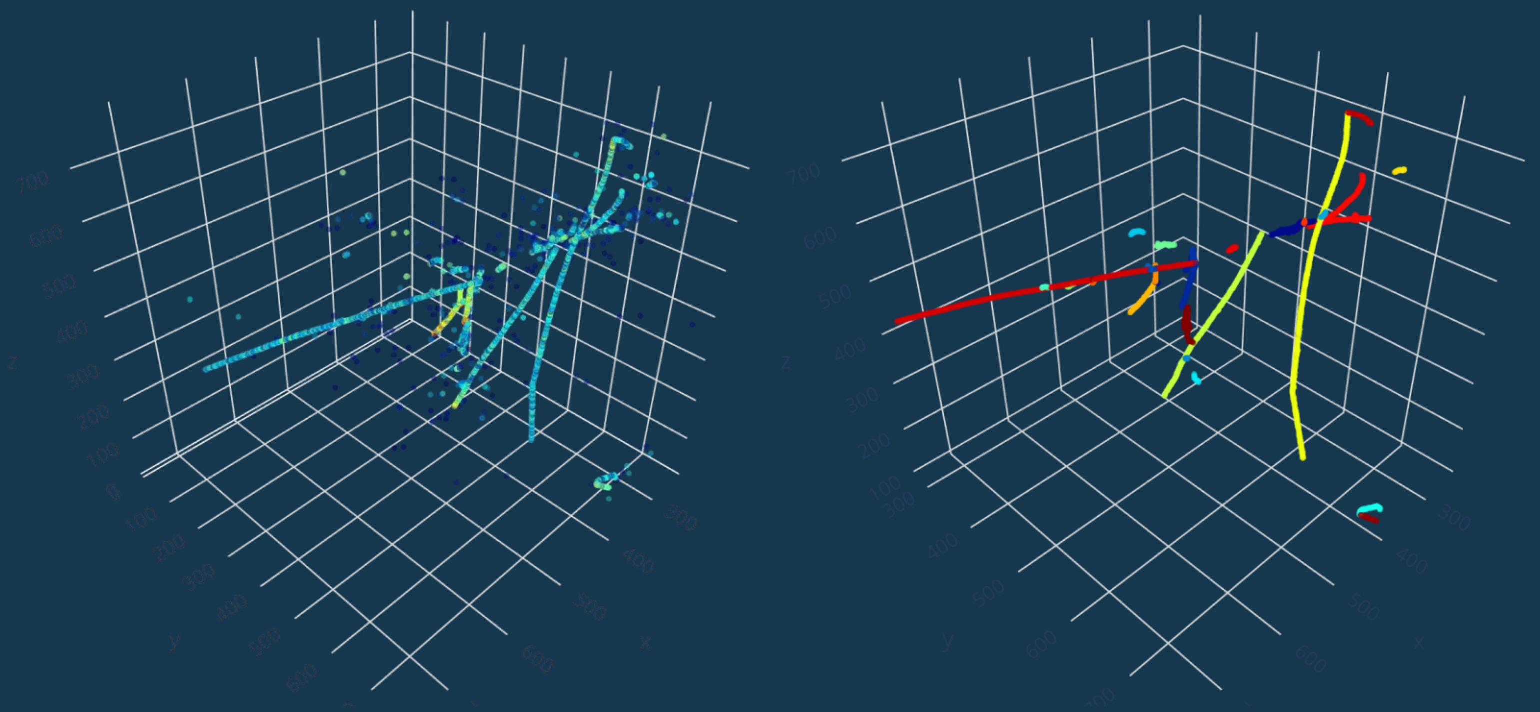

Proposal-free Deep Sparse Convolutional Neural Network for 3D Pixel Clustering

P. Cote de Soux, L. Domine, F. Drielsma, R. Itay, **D. Koh***, Q. Lin, B. Nelson, P. Tsang, K.Terao, T. Usher

U.S. DEPARTMENT OF ENERGY | Office of Science

Stanford University

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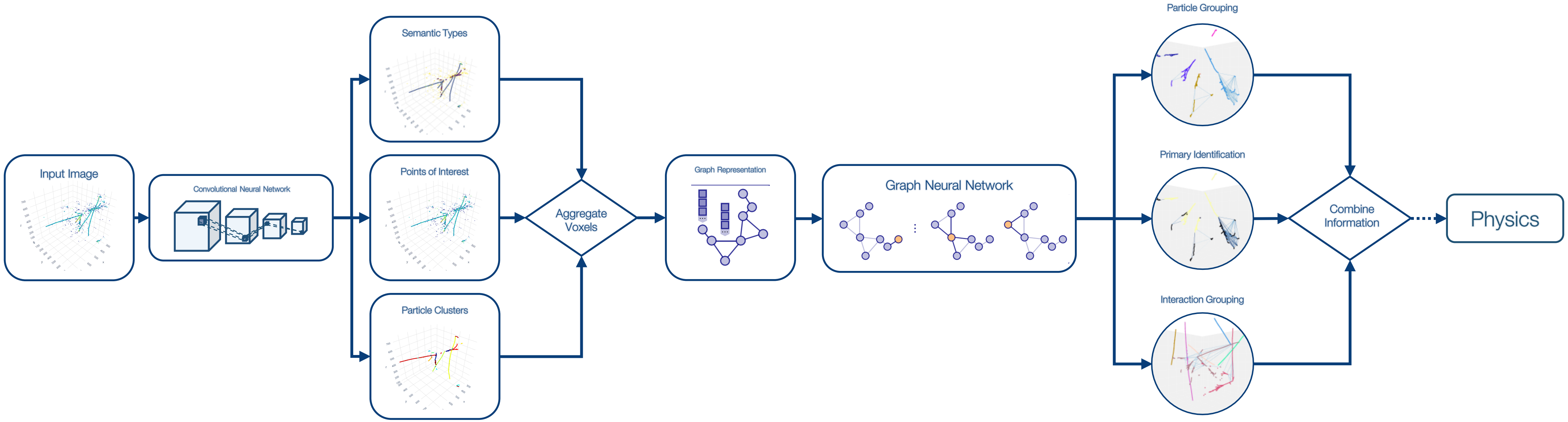
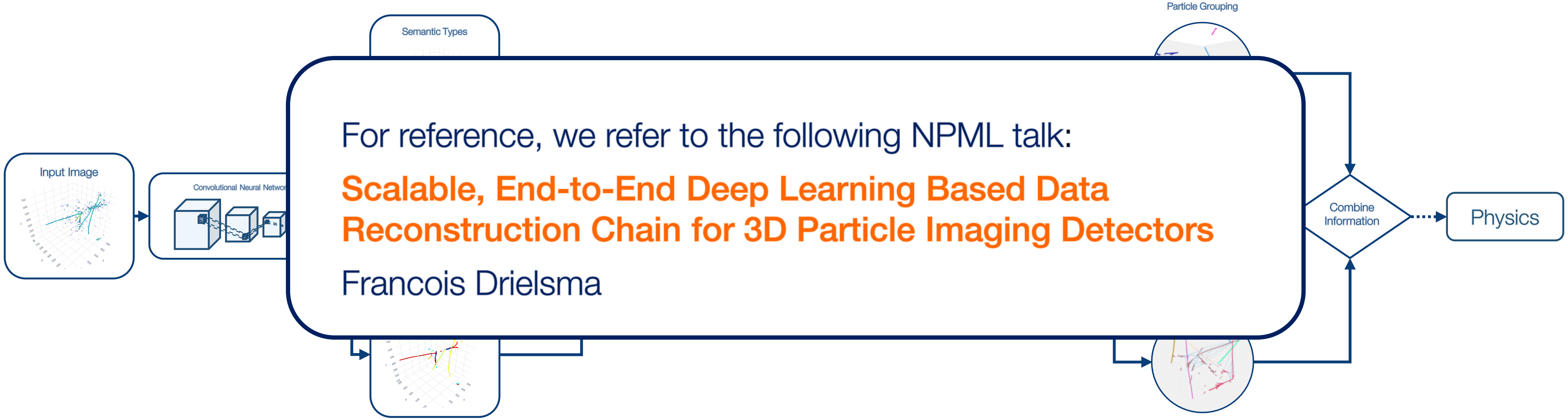
In SLAC, we aim to develop a full ML-based, general purpose reconstruction chain for LArTPC data.



In SLAC, we aim to develop a full ML-based, general purpose reconstruction chain for LArTPC data.



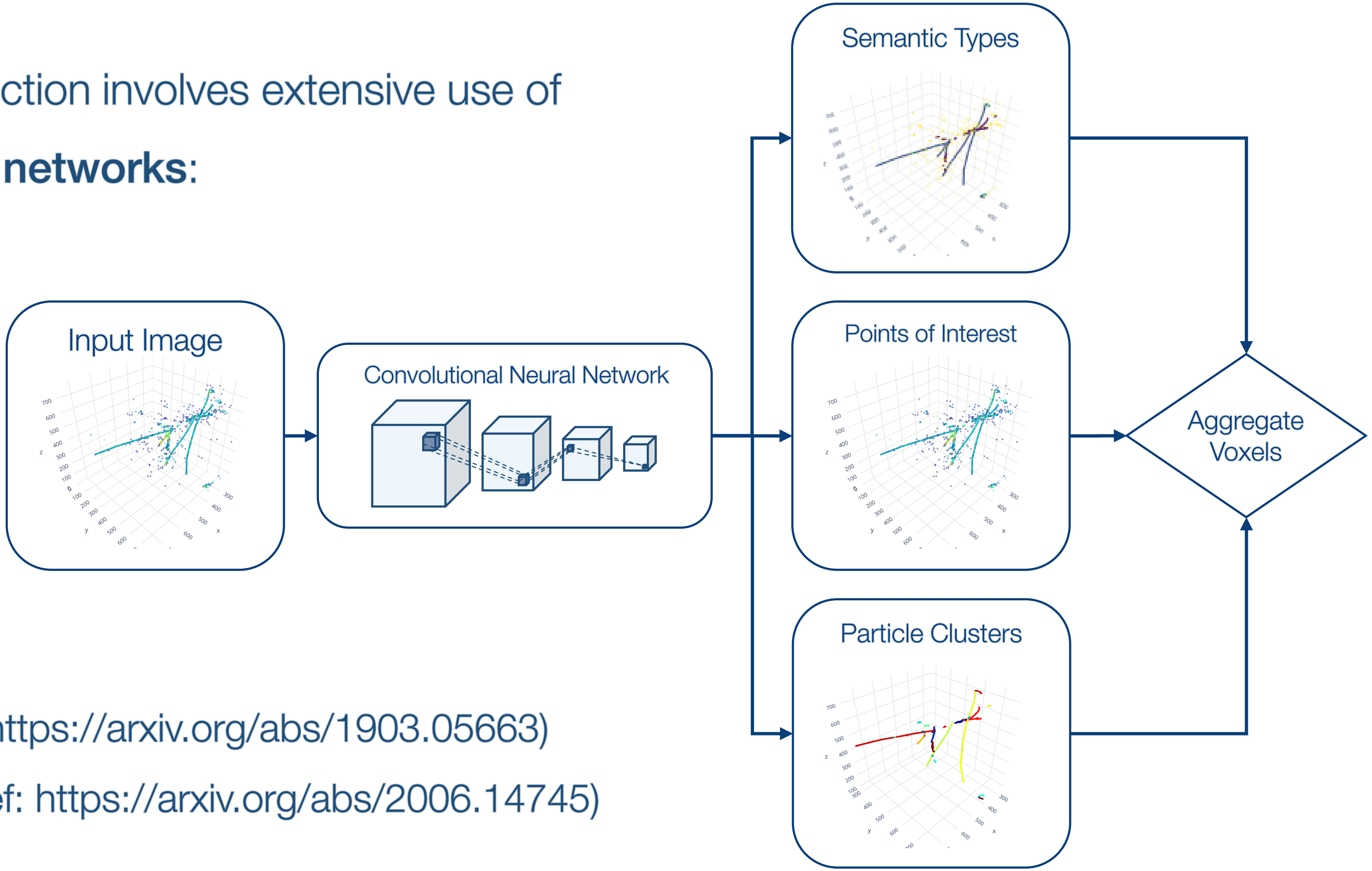
For reference, we refer to the following NPML talk:

Scalable, End-to-End Deep Learning Based Data Reconstruction Chain for 3D Particle Imaging Detectors

Francois Drielsma

SLAC NATIONAL ACCELERATOR LABORATORY

A. The first phase of reconstruction involves extensive use of **sparse convolutional neural networks**:

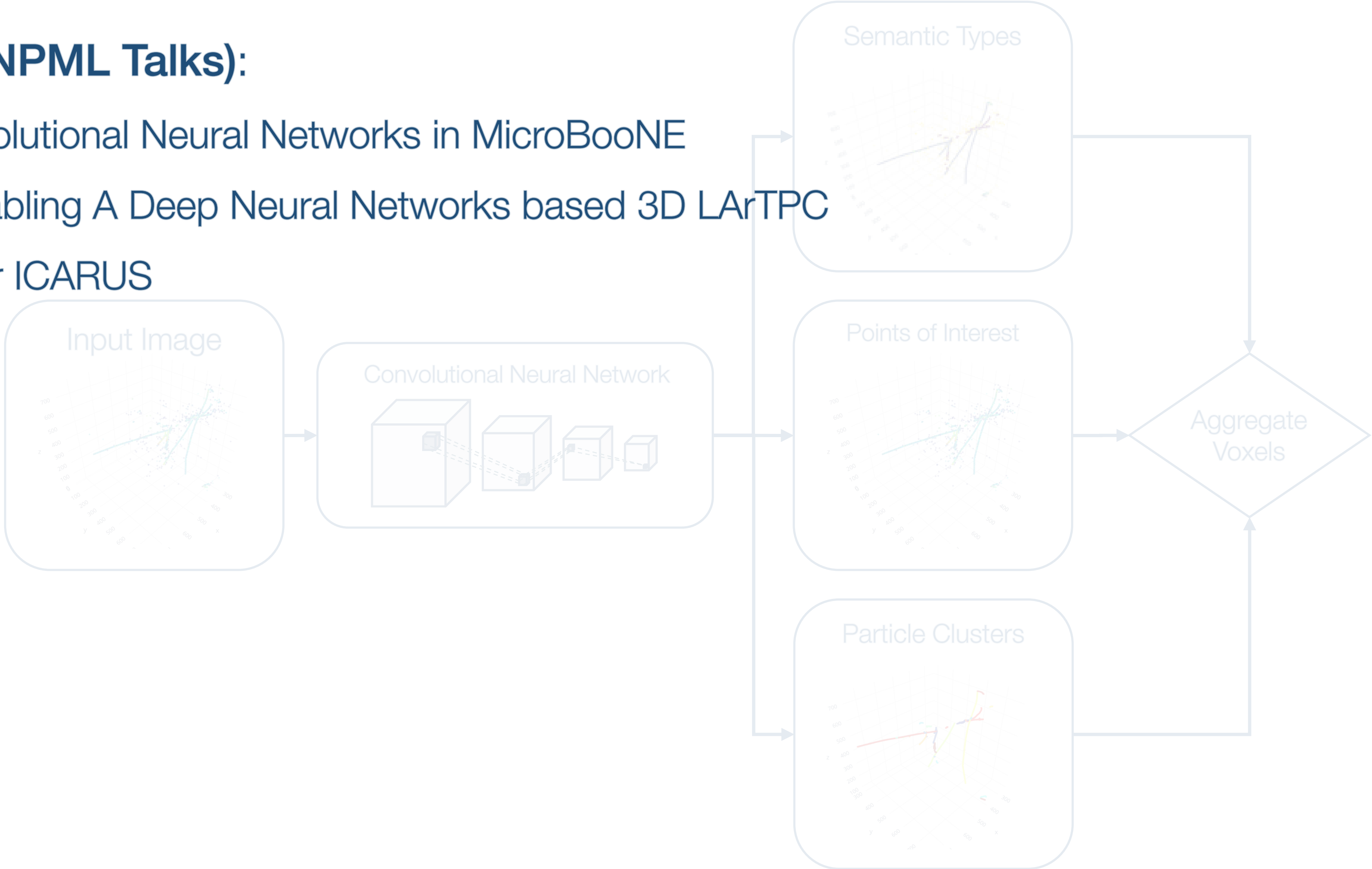


Relevant Work:

- Semantic Segmentation (ref: https://arxiv.org/abs/1903.05663)
- Points of Interest Detection (ref: https://arxiv.org/abs/2006.14745)

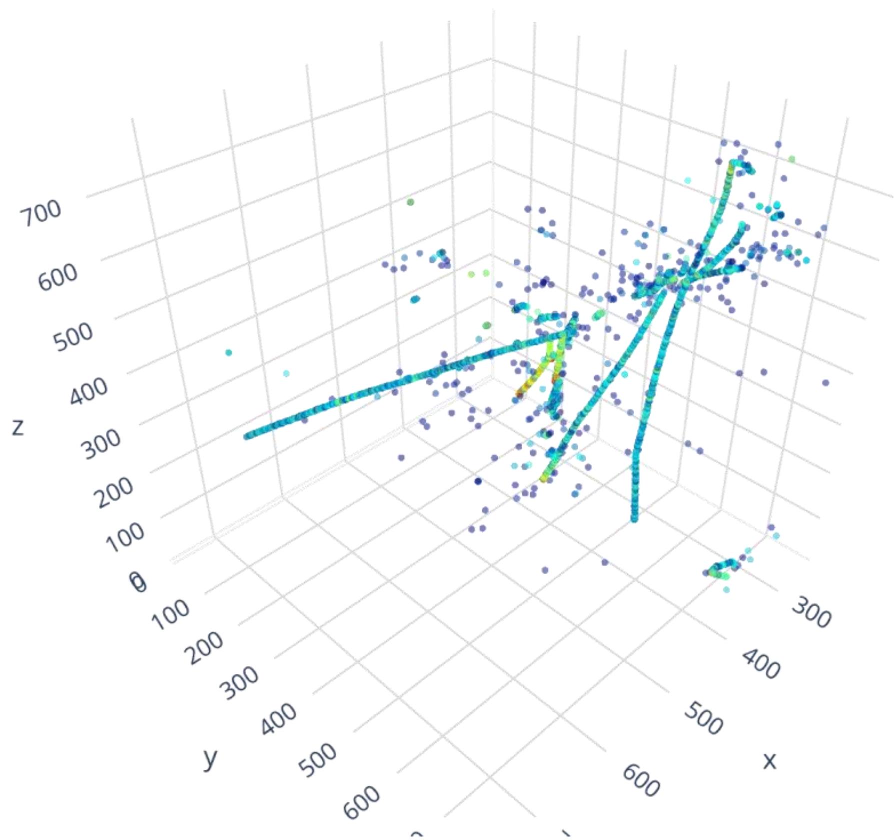
Experimental Applications (NPML Talks):

- **Ran Itay**: Using Sparse Convolutional Neural Networks in MicroBooNE
- **L. Domine and P. Tsang**: Enabling A Deep Neural Networks based 3D LArTPC Data Reconstruction Chain for ICARUS



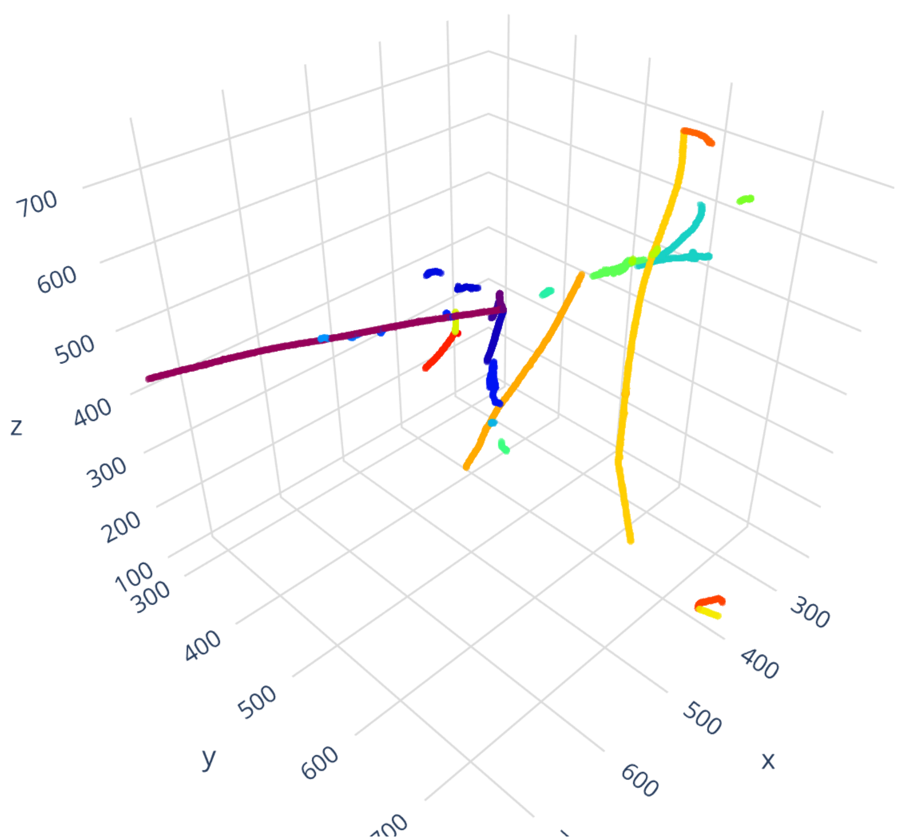
Dense Clustering: cluster voxels that belong to the same particle instance.

Energy Depositions



Remove low-E depositions with semantic labels

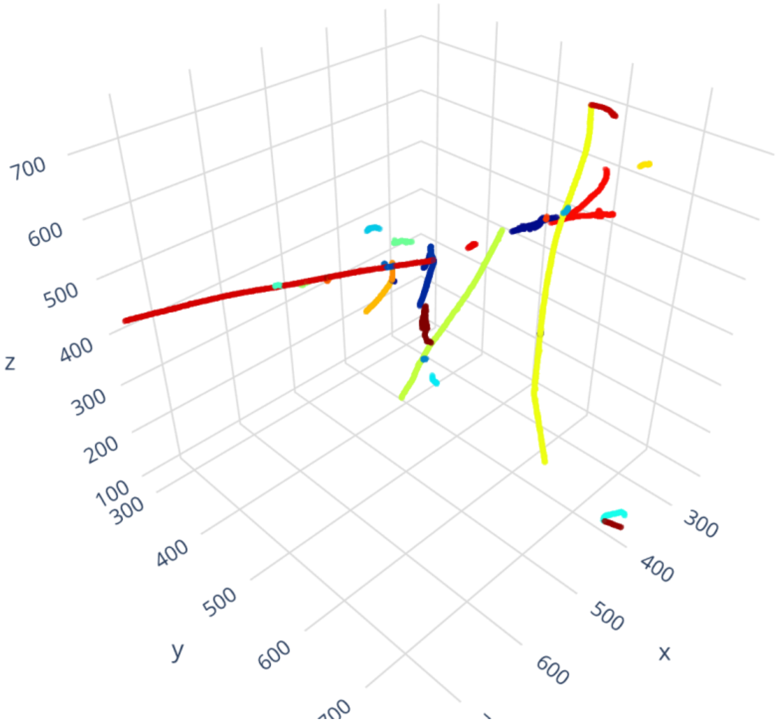
Particle Fragment Labels

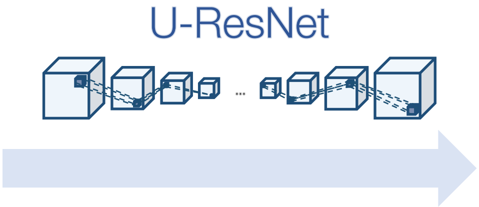


Dense Clustering: cluster voxels that belong to the same particle instance.

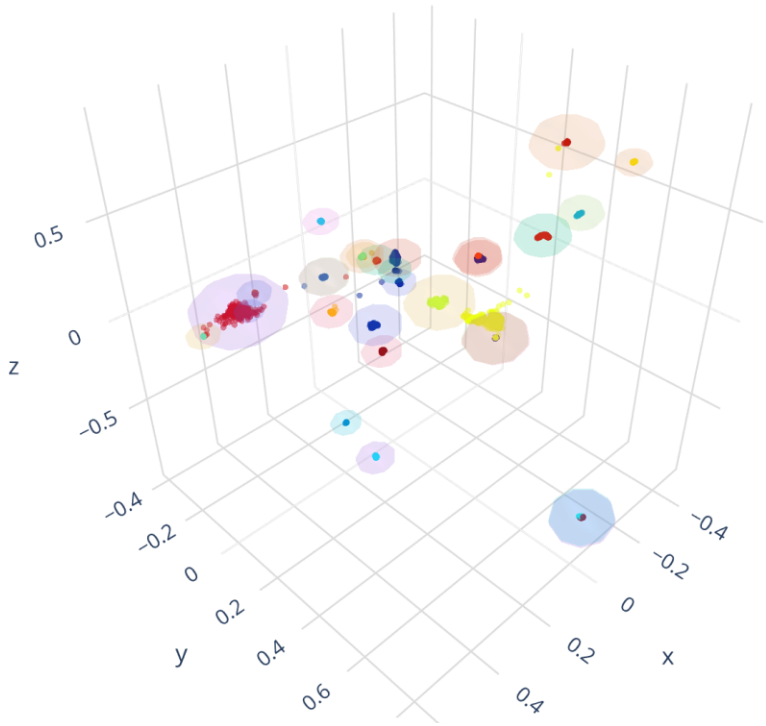
- Supervised training of embedding generation, points that belong to the same particle instance are grouped nearby each other in embedding space

Energy Depositions





Voxel Embeddings



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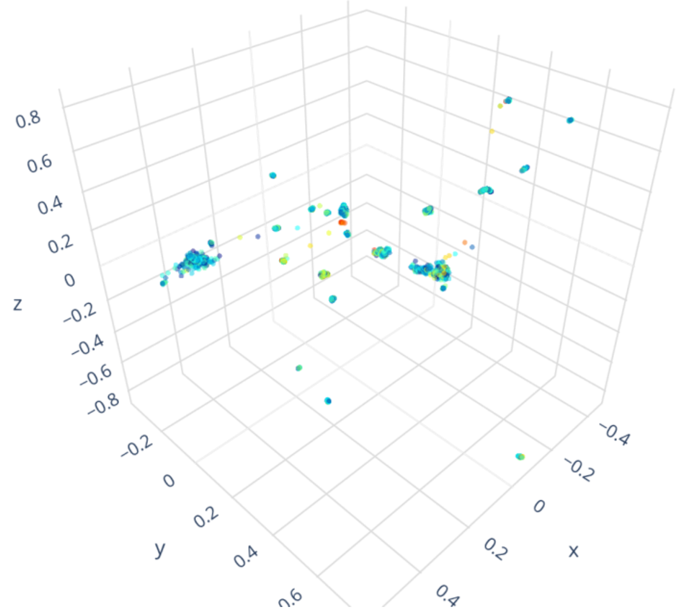
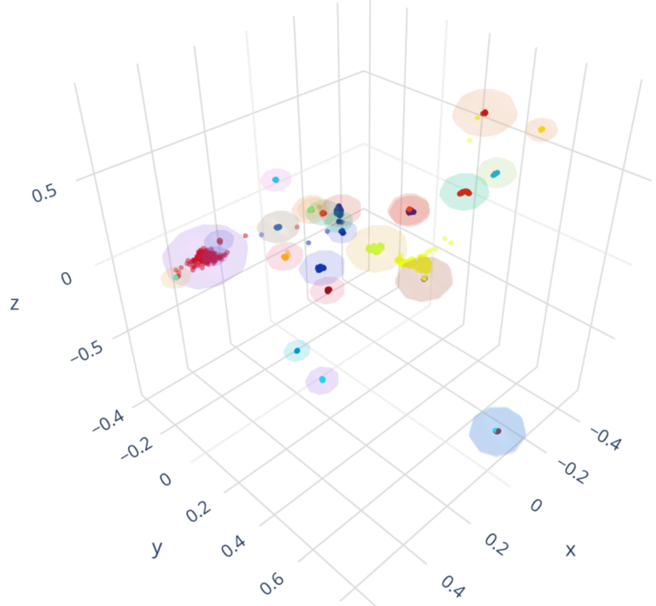
Dense Clustering: cluster voxels that belong to the same particle instance.

- Supervised training of embedding generation, points that belong to the same particle instance are grouped nearby each other in embedding space (ref: D. Koh et. al., https://arxiv.org/abs/2007.03083)
- Run a clustering algorithm on embedding space, generate predicted particle cluster labels

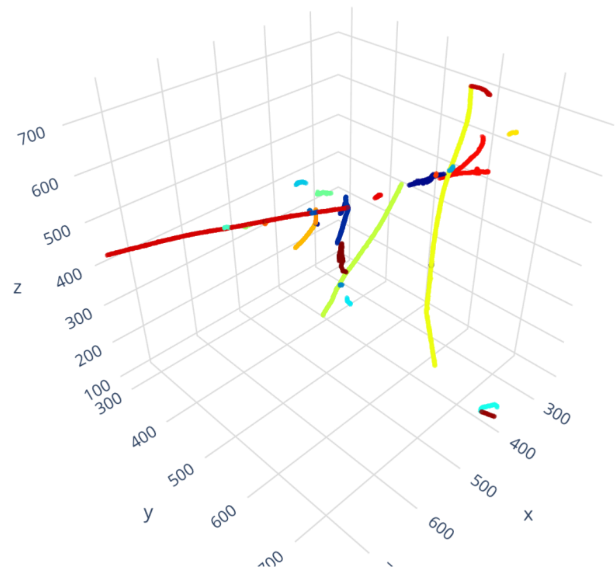
1. Voxel Embeddings



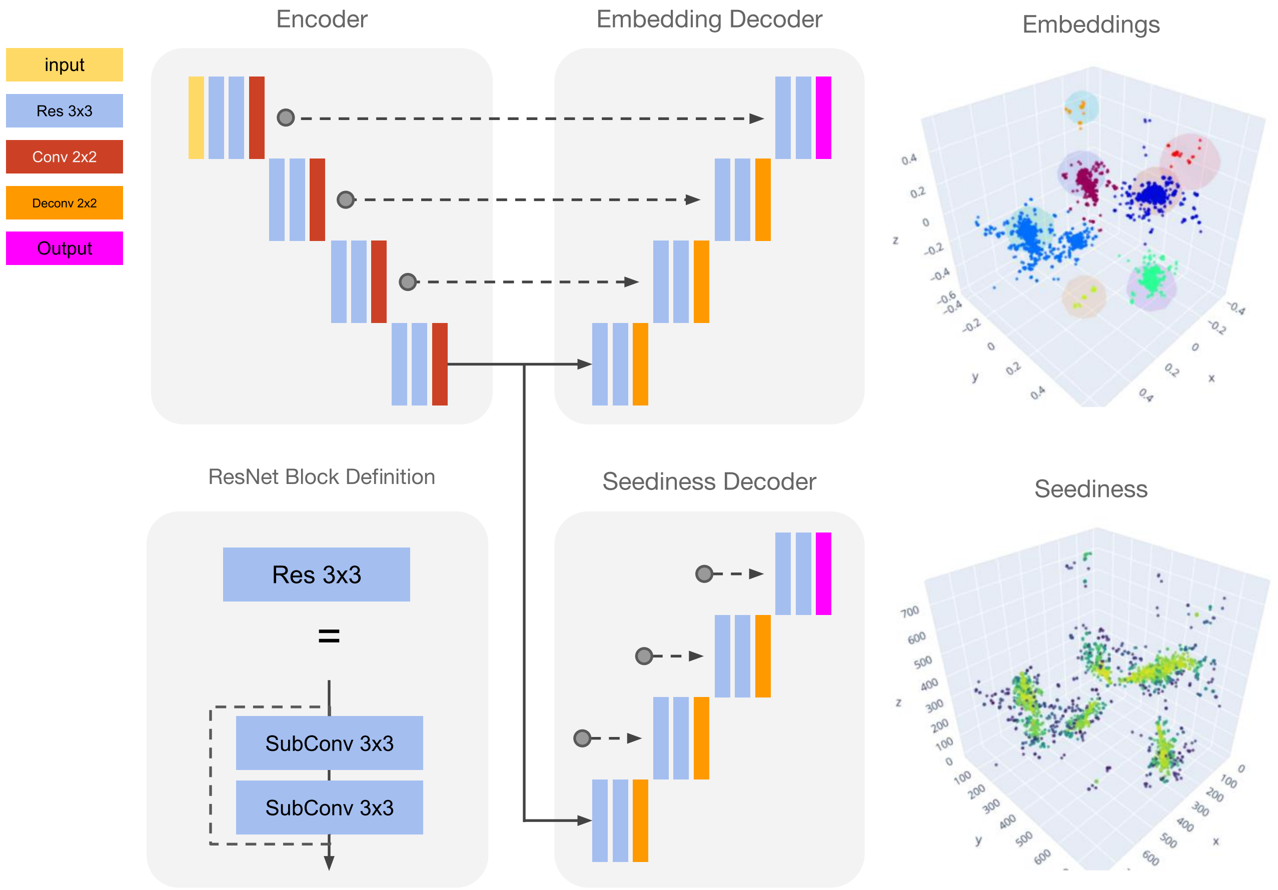
2. Gaussian Kernel Clustering



3. Predicted Cluster Labels



We use a U-ResNet with one shared encoder and two decoders:

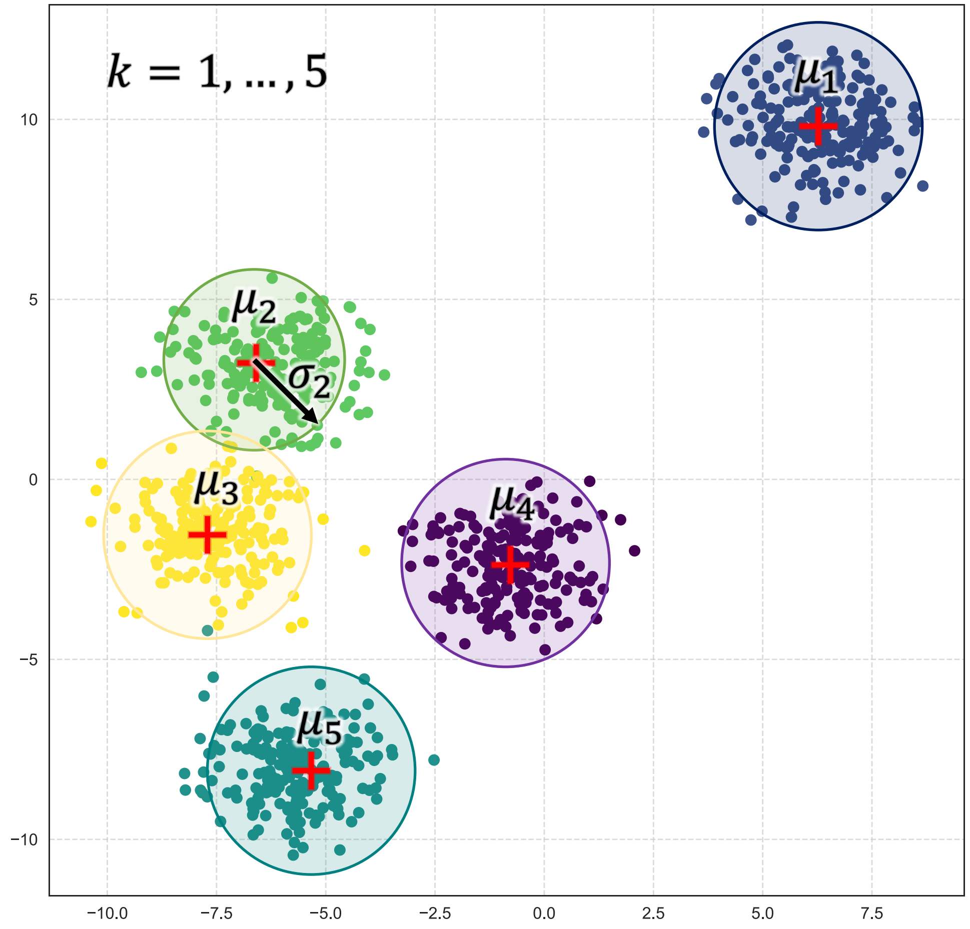


Embeddings: transform image voxel to representation in embedding space, predict size of cluster σ:

$$f_{emb}(x_i) \in [-1, 1]^3, \qquad \sigma(x_i) \in [0,2].$$

Seediness: trained to predict a score between 0 and 1, indicating proximity to embedding space centroid.

$$s_i \equiv s(x_i) \in [0,1].$$



We present a summary of the proposal-free algorithm by D. Neven et. al. (ref: https://arxiv.org/abs/1906.11109)

Training:

- For each true cluster k, compute centroid μ_k and average margin σ_k:

$$\mu_k = \frac{1}{n_k}\sum_{i=1}^{n_k} f_{emb}(x_i), \qquad \sigma_k = \frac{1}{n_k}\sum_{i=1}^{n_k} \sigma(x_i).$$

Note: Following scatterplots are for illustration purposes only.

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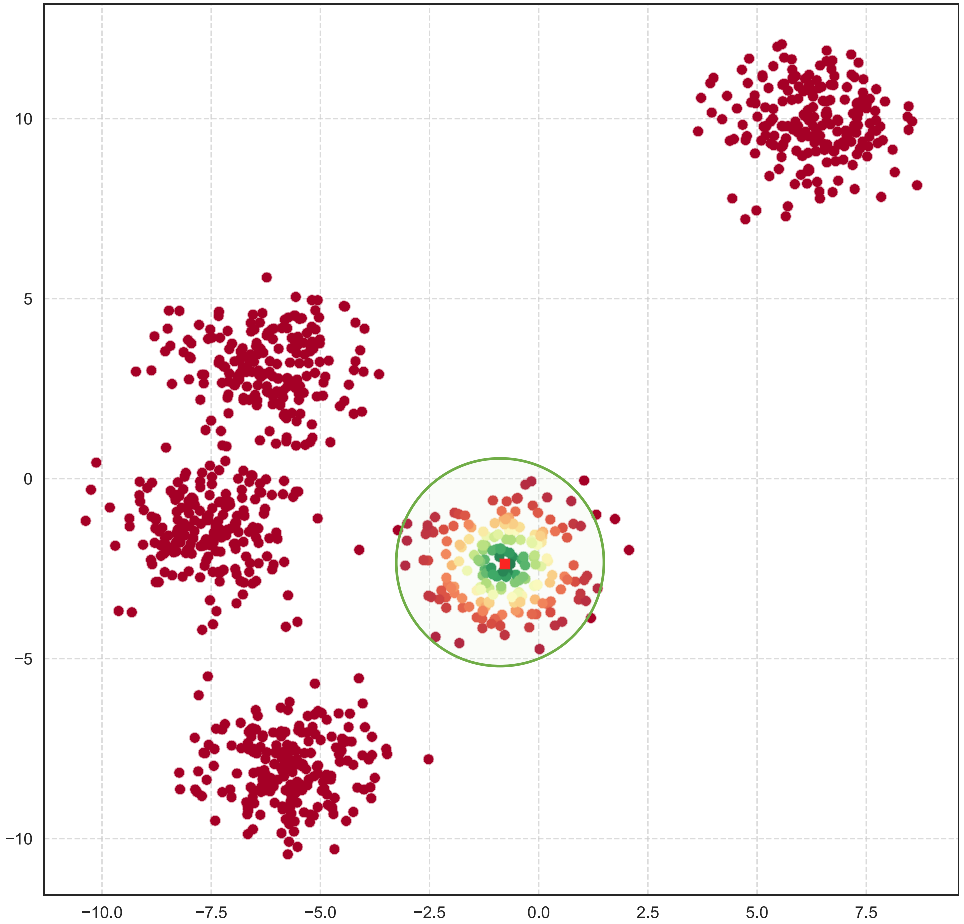

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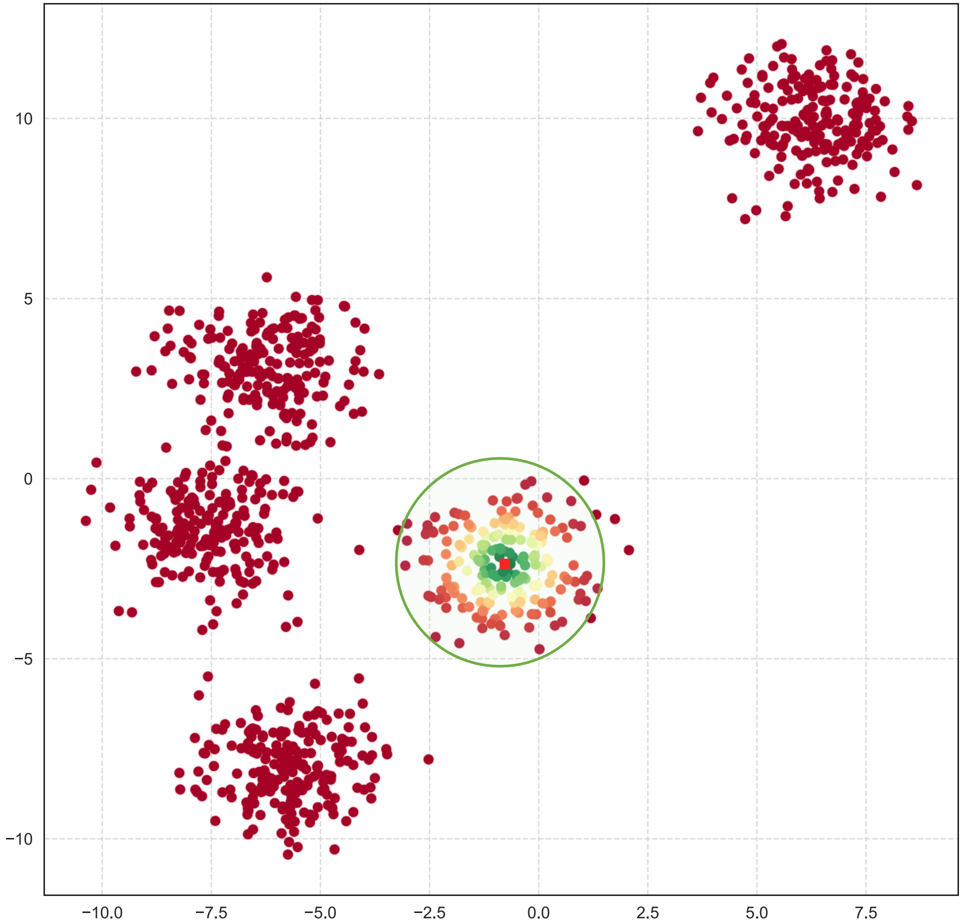
- Define a kernel map $p(\cdot\,; \mu_k, \sigma_k)$, where:

$$p(x; \mu_k, \sigma_k) = \exp\left(-\frac{\left|\left|f_{emb}(x_i) - \mu_k\right|\right|^2}{2\sigma_k^2}\right).$$



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- For each true cluster k, compute **centroid** μ_k and average **margin** σ_k:

$$\mu_k = \frac{1}{n_k}\sum_{i=1}^{n_k} f_{emb}(x_i), \qquad \sigma_k = \frac{1}{n_k}\sum_{i=1}^{n_k} \sigma(x_i).$$

- Define a kernel map $p(\cdot\,; \mu_k, \sigma_k)$, where:

$$p_{ik} \equiv p(x_i; \mu_k, \sigma_k) = \exp\left(-\frac{\|f_{emb}(x_i) - \mu_k\|^2}{2\sigma_k^2}\right).$$

- Now problem is a binary classification over scores p:

$$L_{emb}(x_{ik}) = y_{ik}\log(p_{ik}) + (1 - y_{ik})\log(1 - p_{ik}).$$

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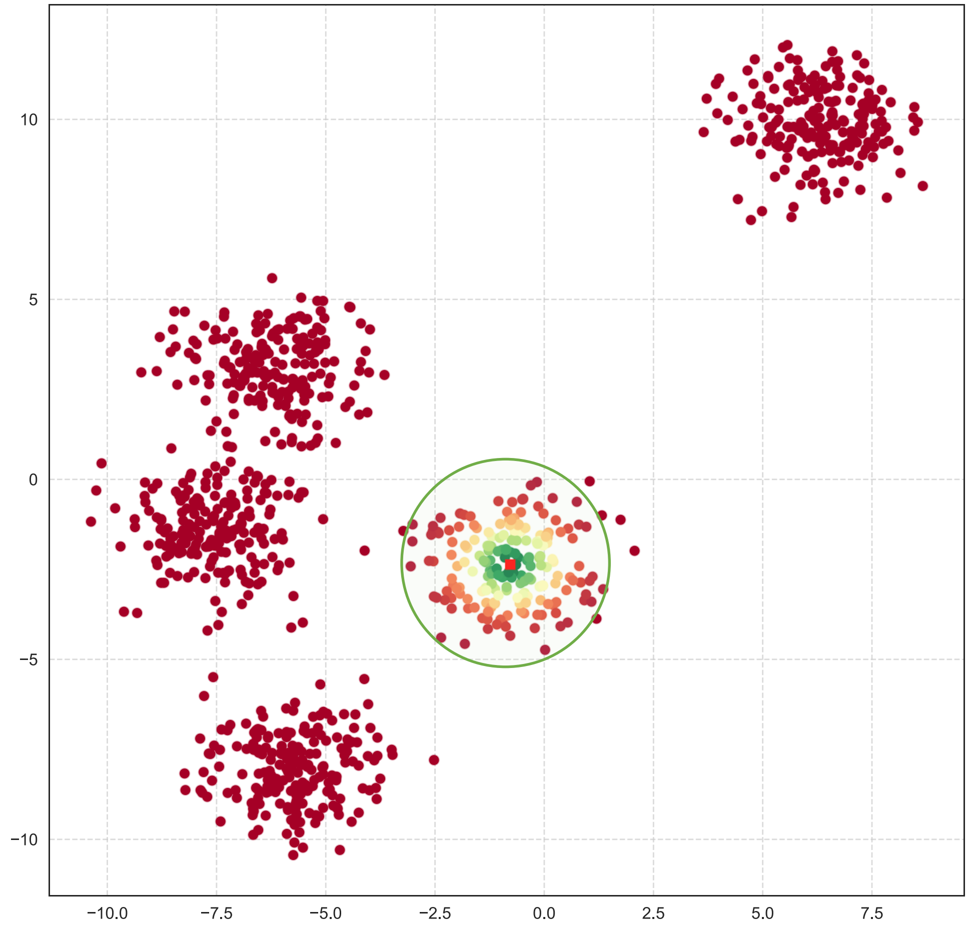


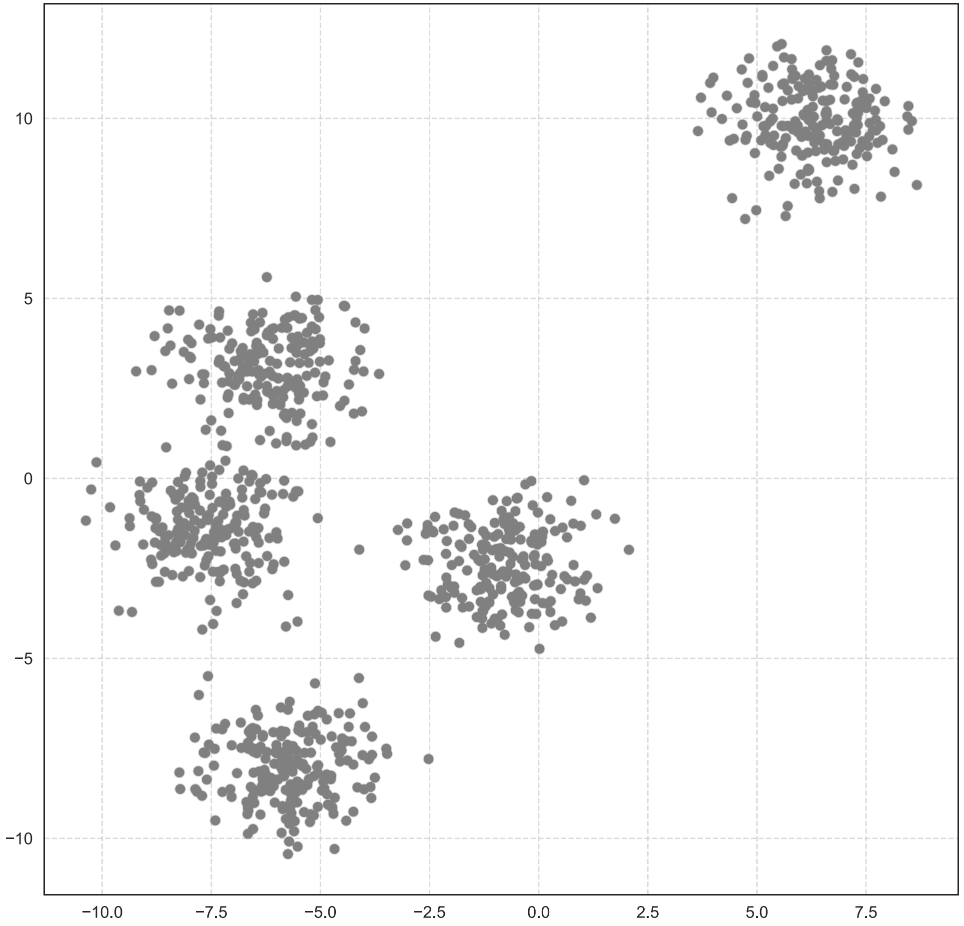
Training:

- Observe that the kernel score give a proximity score towards the centroid:

$$p_{ik} \equiv p(x_i; \mu_k, \sigma_k) = \exp\left(-\frac{||f_{emb}(x_i) - \mu_k||^2}{2\sigma_k^2}\right).$$

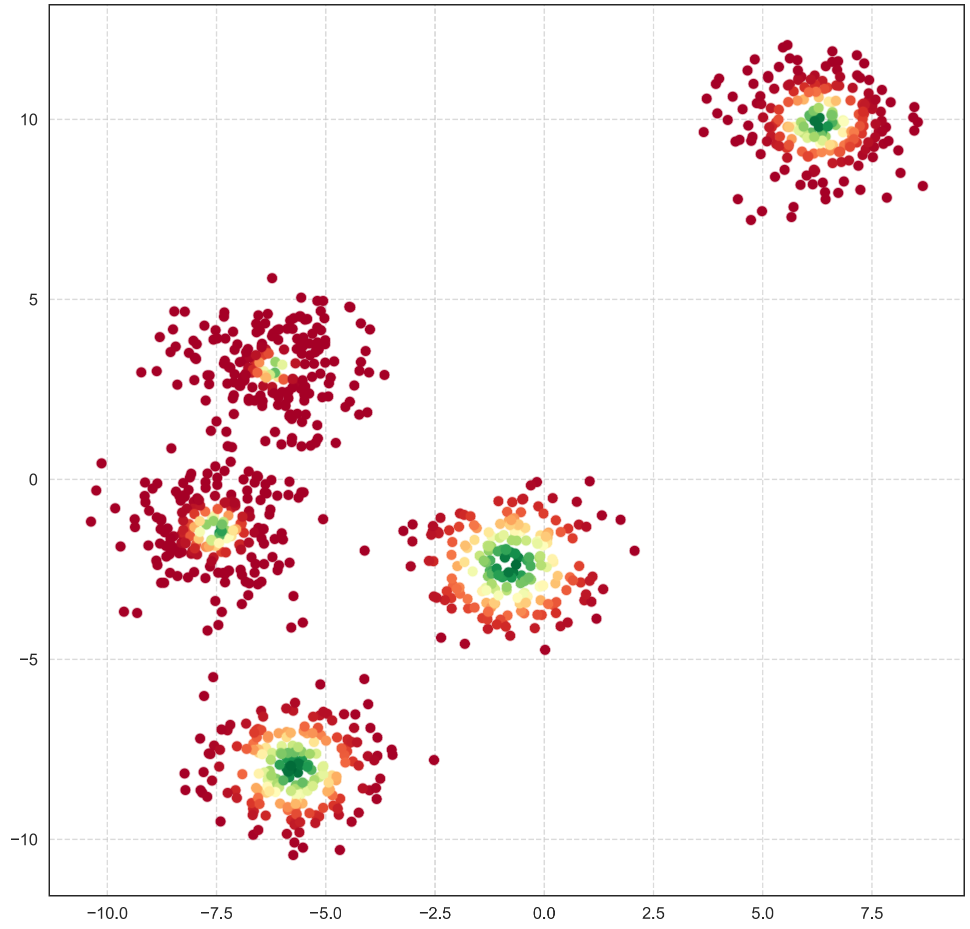
- To train seediness, we simply take p_{ik} as truth and supervise seediness branch to predict p_{ik}:

$$L_{seed}(x_i) = ||s(x_i) - p_{ik}||^2$$



Inference:

- At inference time, we do not have labels to define the centroids μ_k and margins σ_k.



Inference:

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- The **seediness** predictions s_i (color) indicate likely candidates for cluster centroids.

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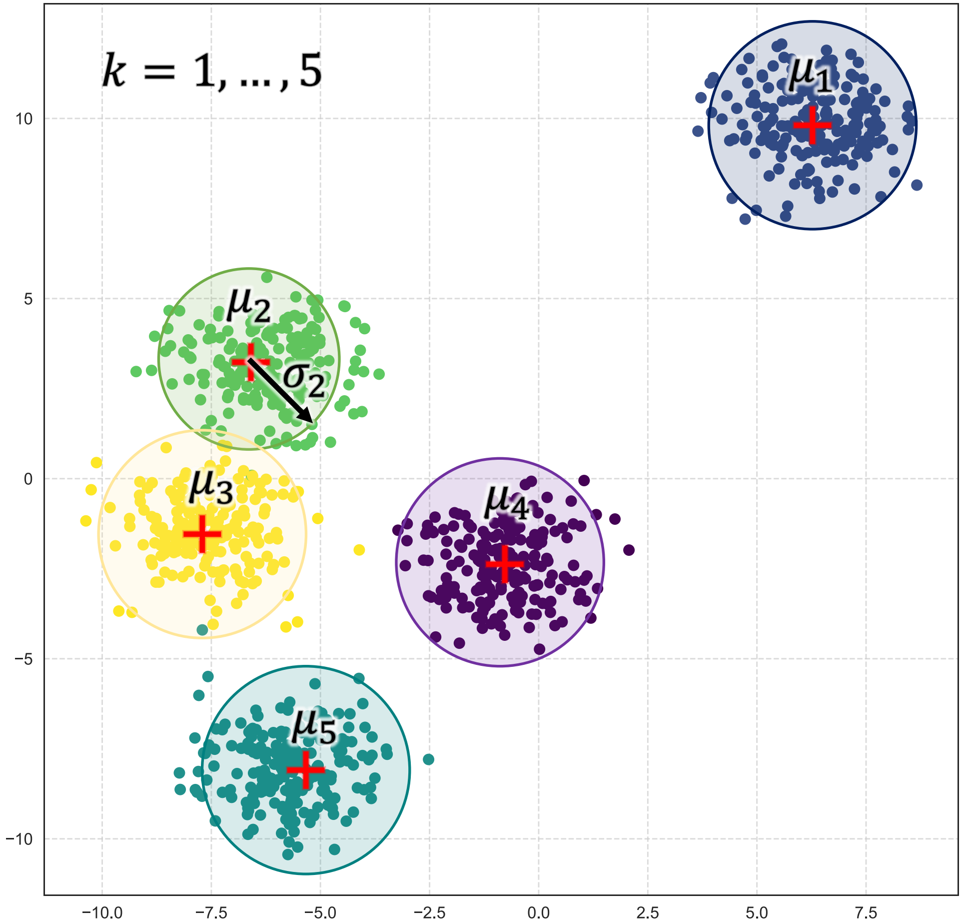
- The **seediness** predictions s_i (color) indicate likely candidates for cluster centroids.
- Start from highest seediness point as μ_k, and assign embeddings to cluster k by thresholding on kernel score p_{ik}.



Inference:

- At inference time, we do not have labels to define the centroids μ_k and margins σ_k.
- The **seediness** predictions s_i (color) indicate likely candidates for cluster centroids.
- Start from highest seediness point μ_k, and assign embeddings to cluster k by thresholding on kernel score p_{ik}.
- Repeat until either:
  - All voxel have been clustered
  - Seediness goes below a threshold value s_0.

- Train and evaluate network on Monte-Carlo generated open dataset (PILArNet: https://arxiv.org/abs/2006.01993)
- Dataset (https://osf.io/6gvf4/): 80k Training set,~20k validation set.
- Mean Adjusted Rand Index (ARI) = **0.973**

	Shower Fragments	Tracks	Michel electrons	Delta Rays
Average # per Event	15 ± 9	6 ± 3	1 ± 1	5 ± 3
Voxel Counts	21.4M	47.7M	0.793M	1.11M
Percentage of Particle Instances	57%	25%	3%	15%

- Use ground truth semantic labels and cluster within each semantic class.
- Mean Purity and Efficiency are above **99%**

	Shower Fragments	Tracks	Michel electrons	Delta Rays
ARI	0.968	0.961	0.998	0.978
Purity	0.997	0.988	0.999	0.992
Efficiency	0.996	0.983	1.000	0.998
SBD	0.978	0.717	0.998	0.982

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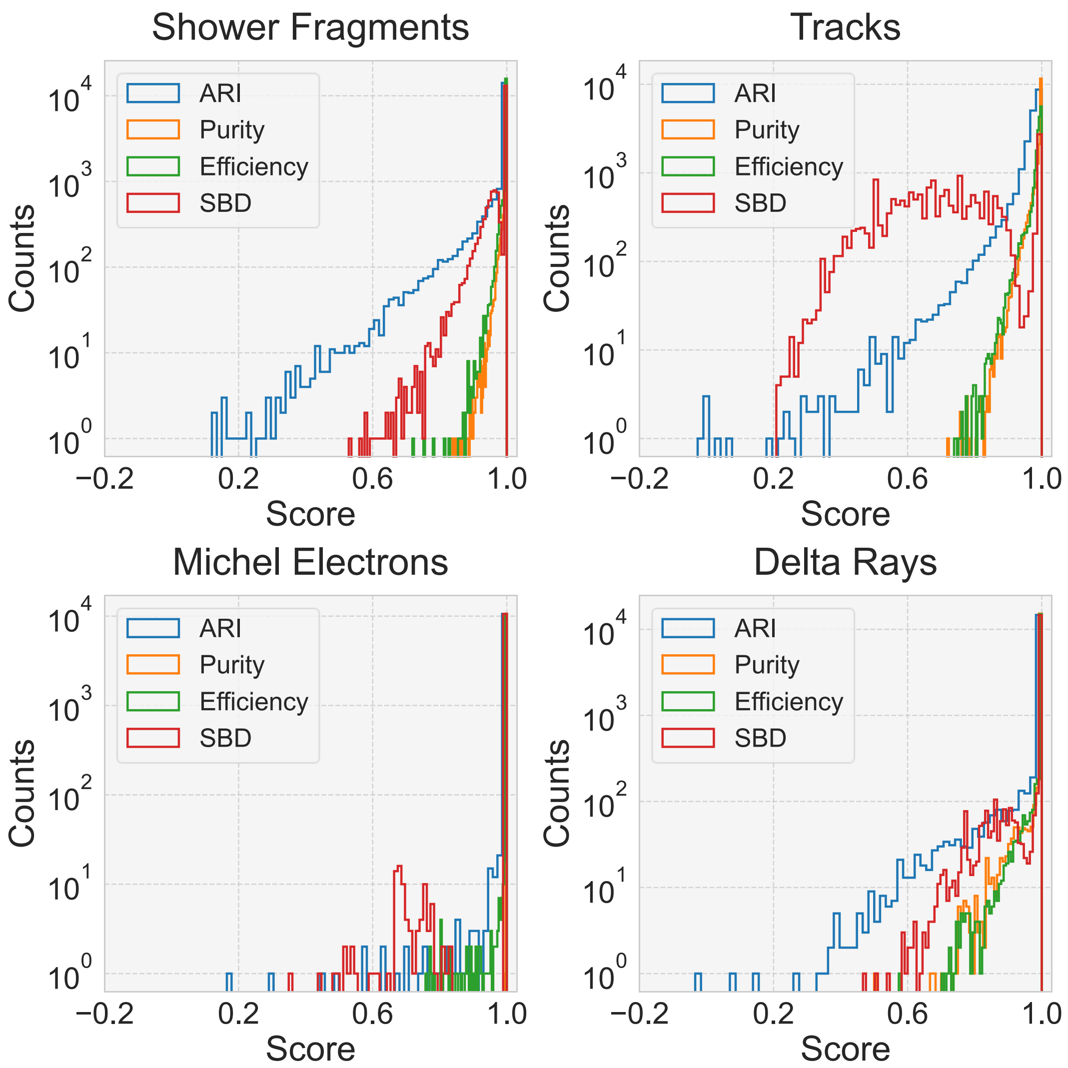

III. Results

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- Use ground truth semantic labels and cluster within each semantic class.
- Mean Purity and Efficiency are above **99%**
- Mean ARI = **0.973**

	Shower Fragments	Tracks	Michel electrons	Delta Rays
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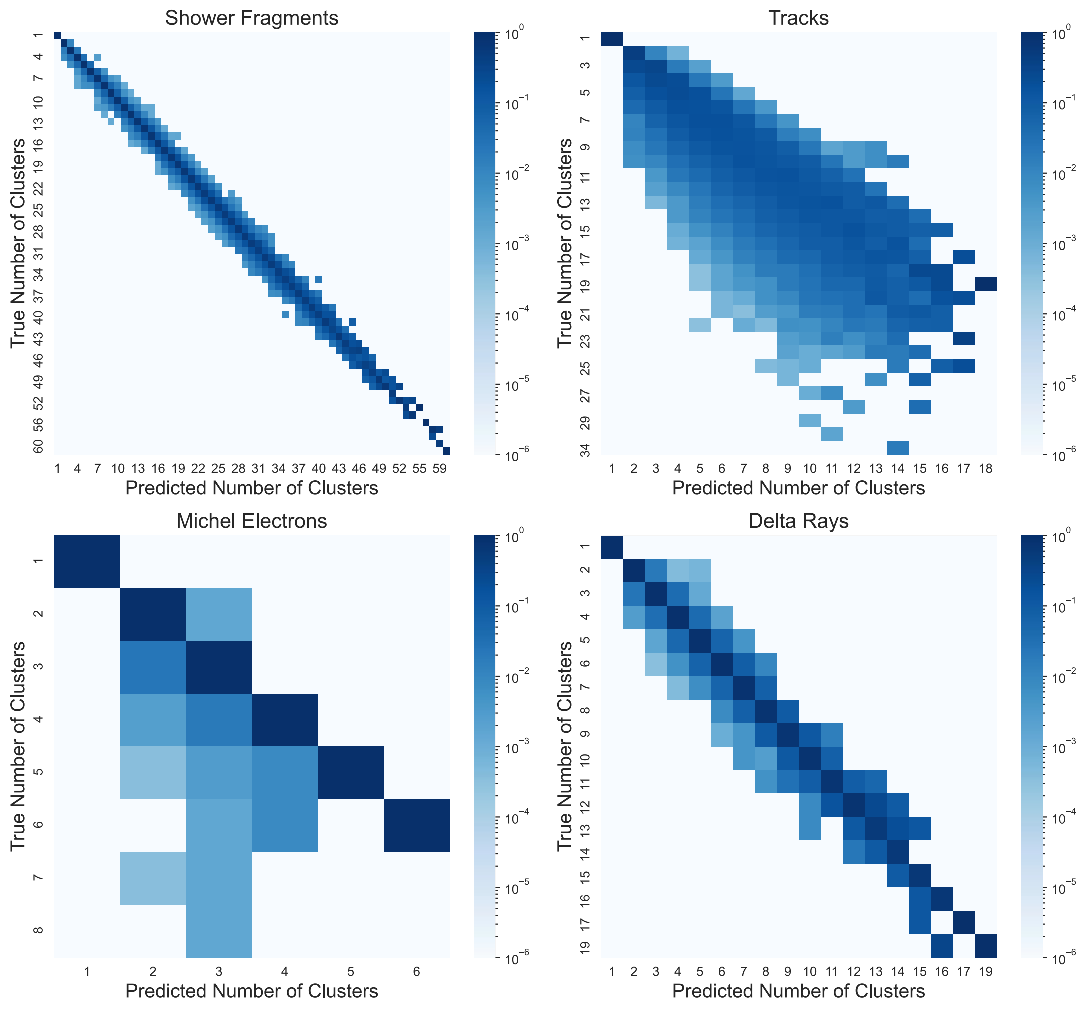
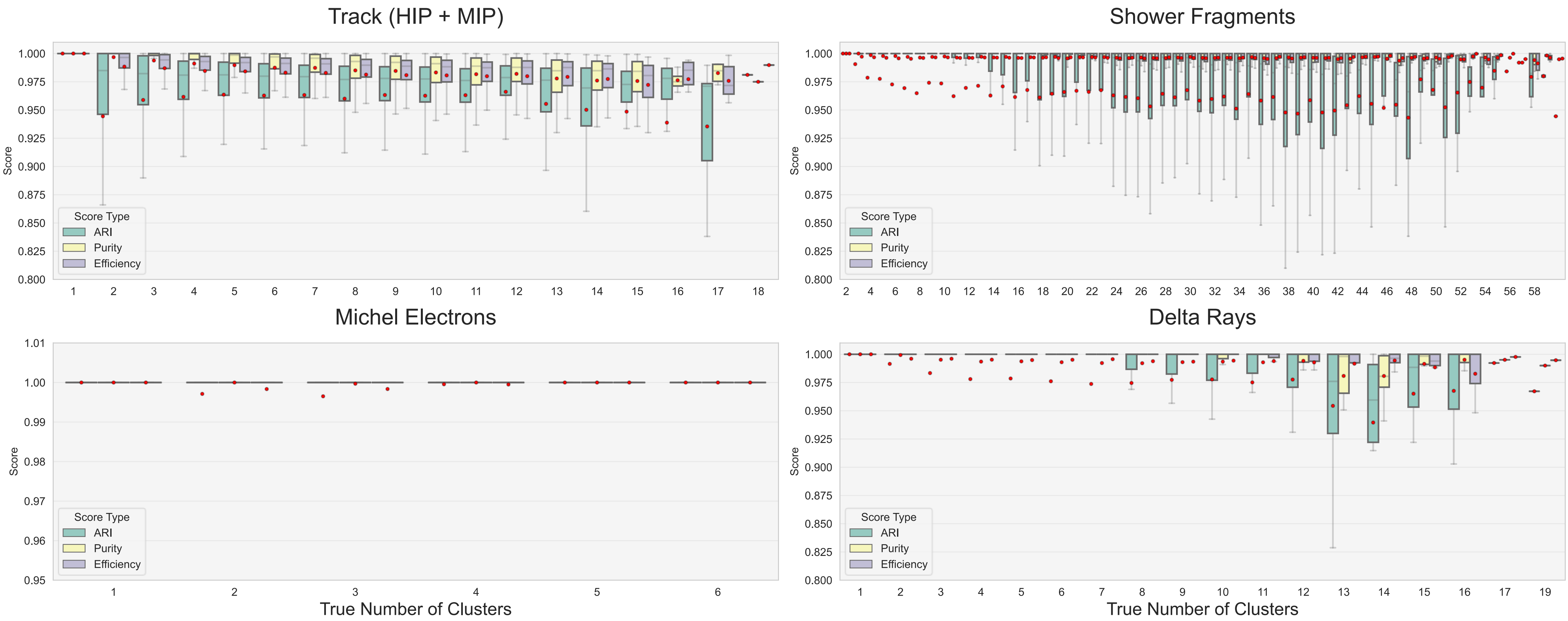


- Some performance degradation towards higher number of particles, yet averaged values are roughly stable.



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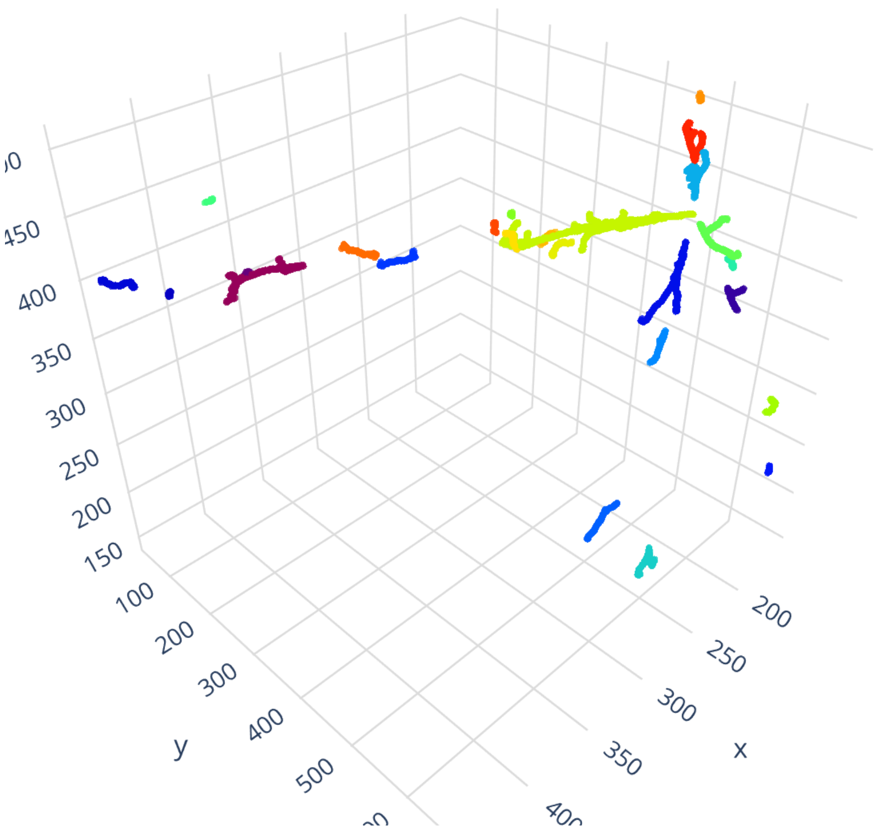
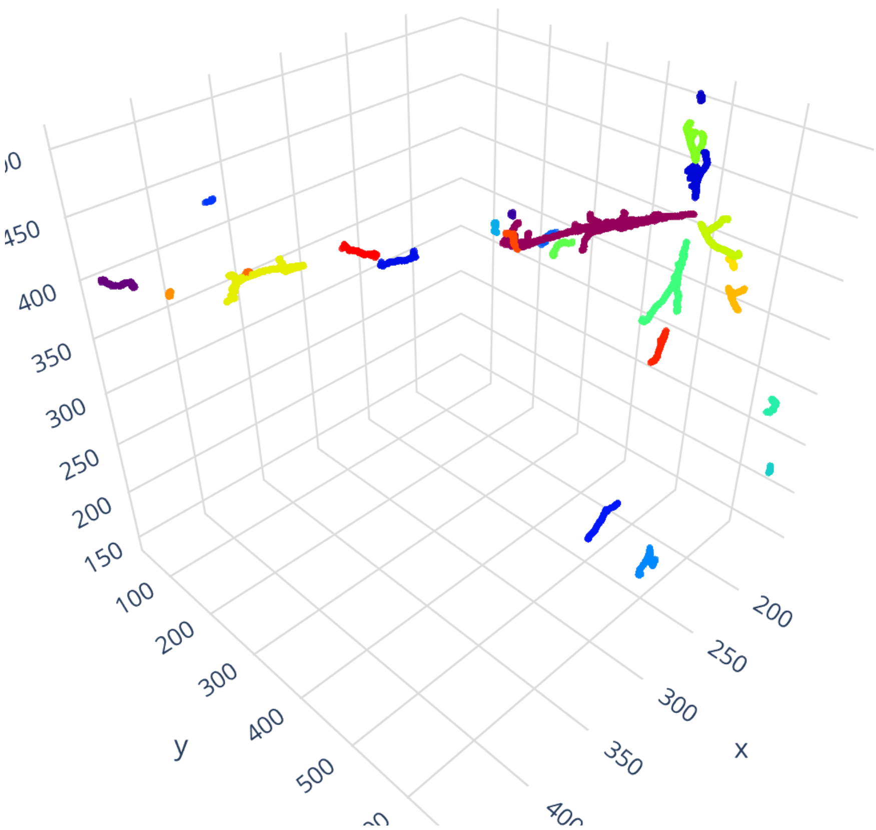
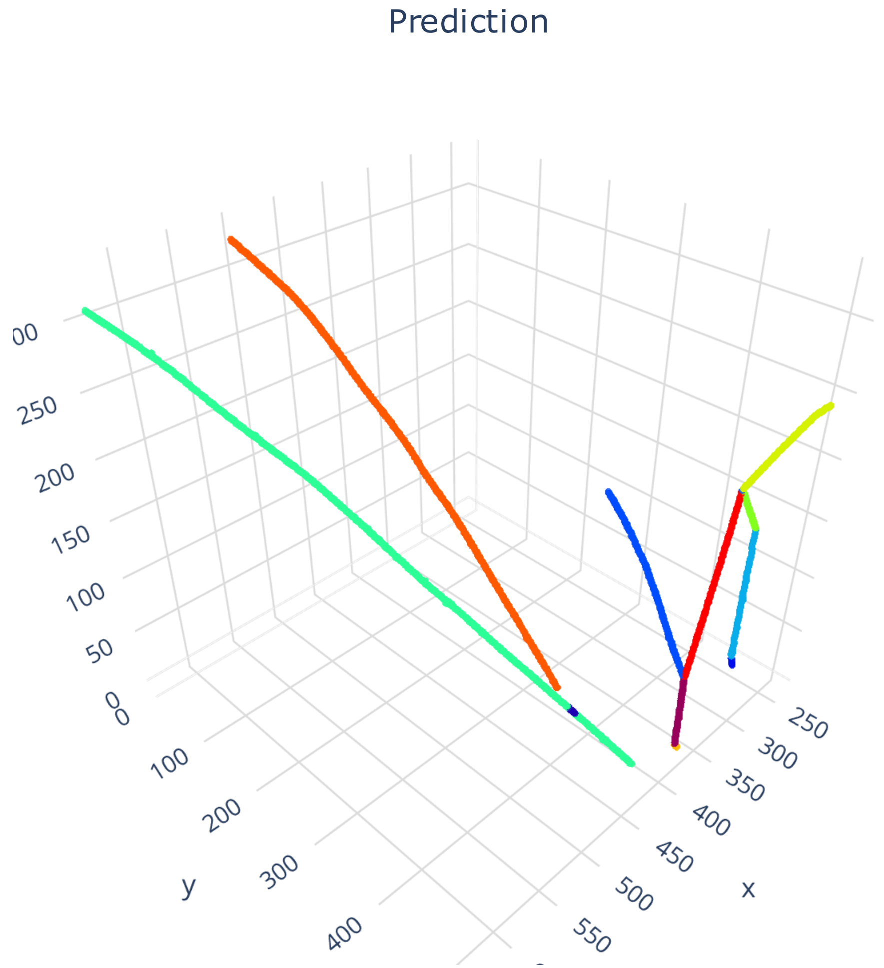
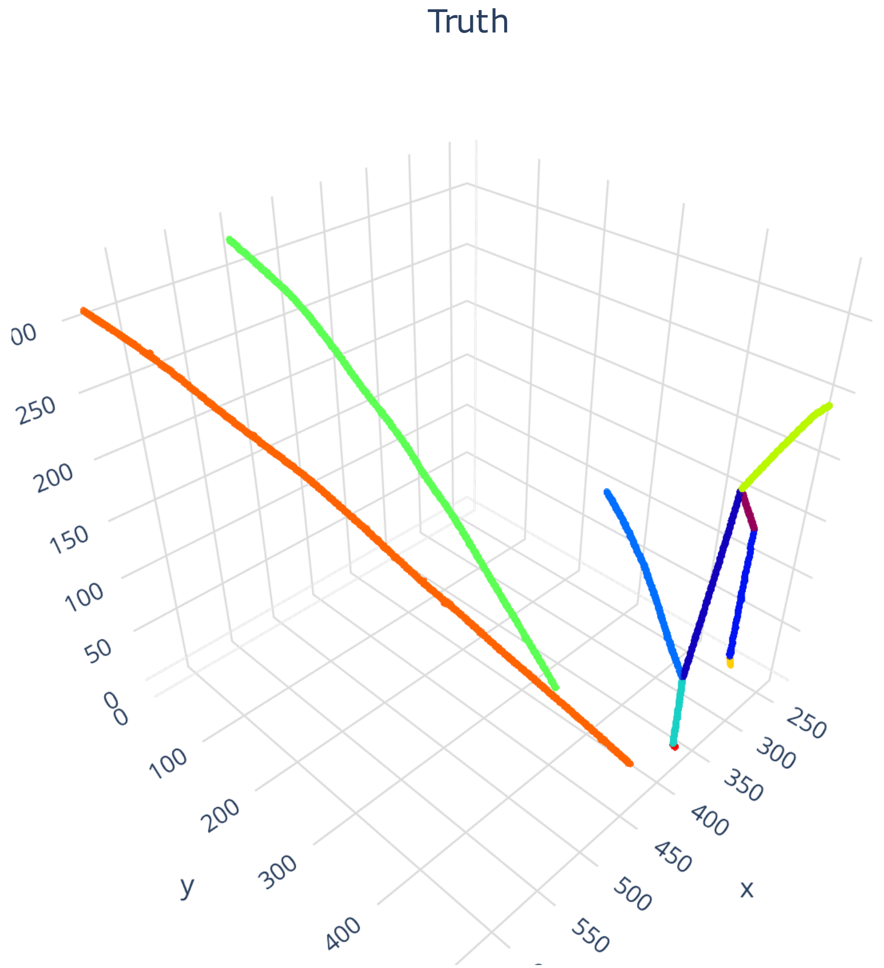
Prediction



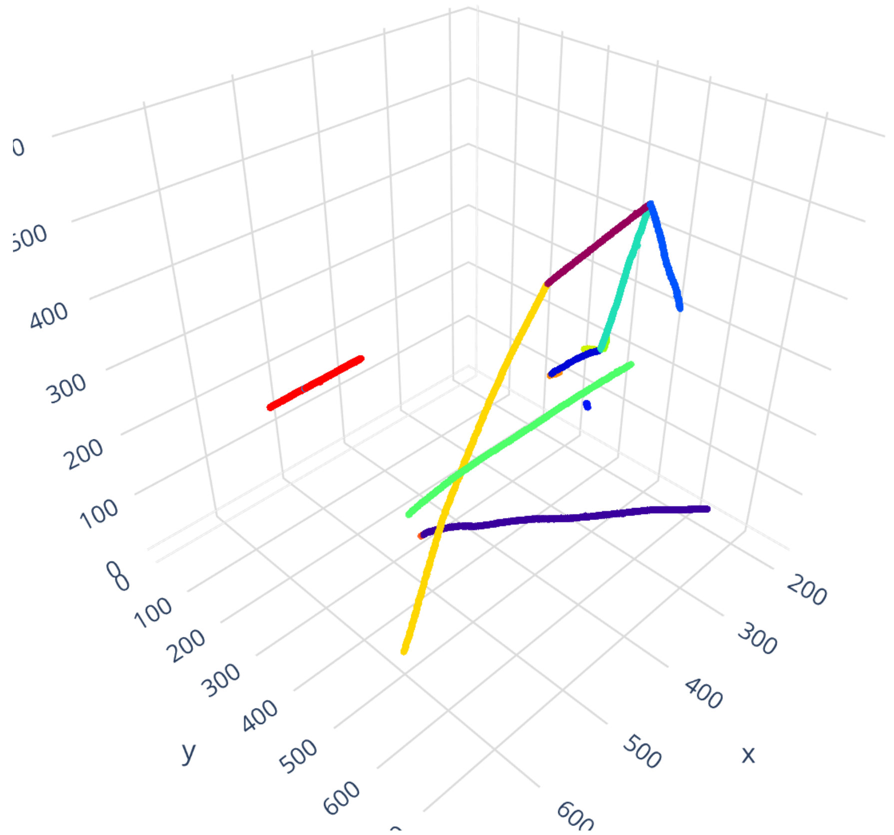
Truth



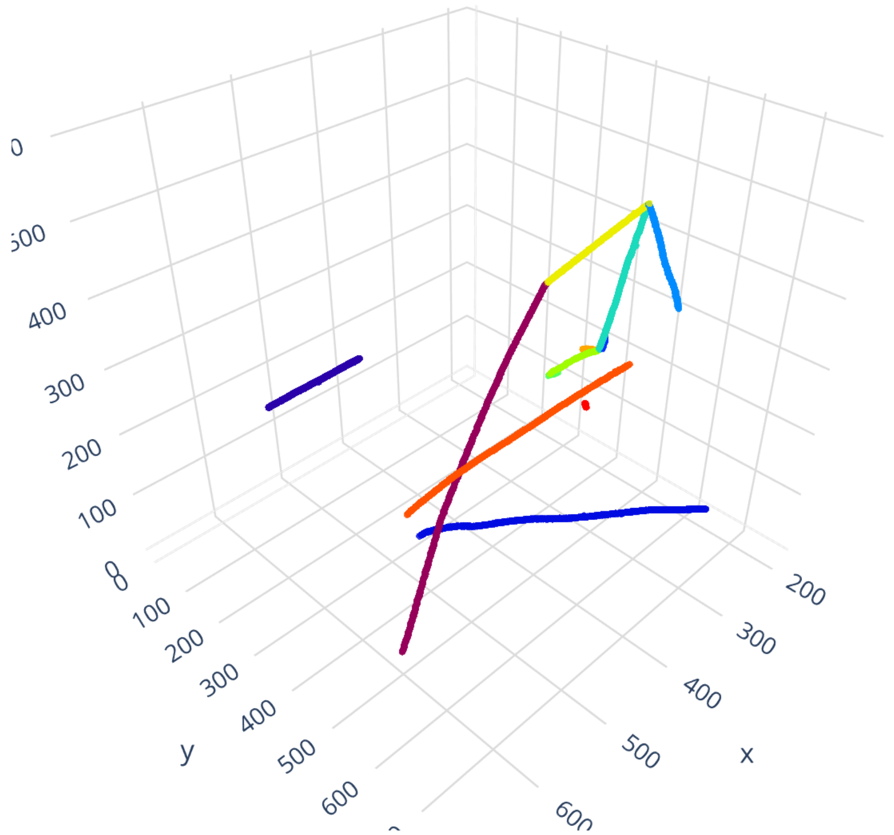

Prediction
00
250
200
150
100
50
0
0
100
200
300
400
y
250
300
350
400
450
500
550
x


Truth
00
250
200
150
100
50
0
0
100
200
300
400
y
250
300
350
400
450
500
550
x

Prediction



Truth



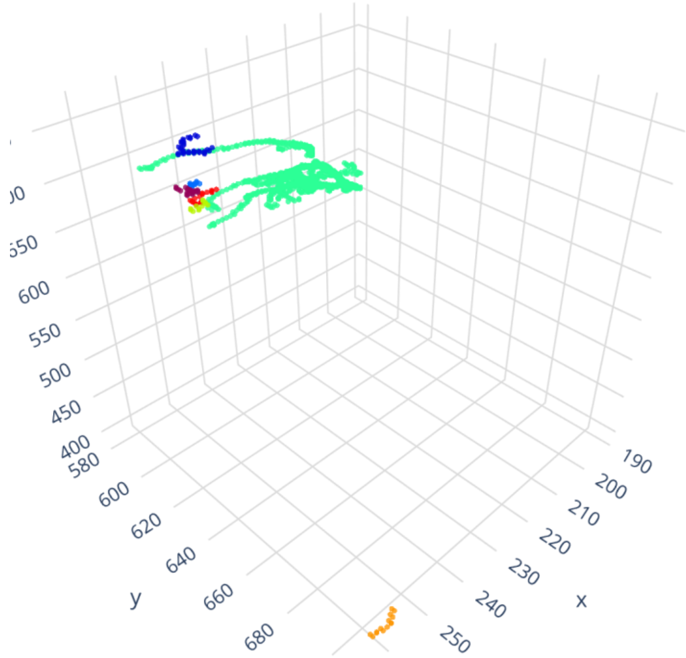
V. Conclusion

- We present a first application of proposal-free instance segmentation network to particle clustering in LArTPCs.
- Further details may be found in the arxiv preprint: D. Koh et. al., https://arxiv.org/abs/2007.03083
    - Results reproducible using Singularity containers and open github repository[1]
- Algorithm relies on accurate semantic segmentation by U-ResNet:
    - L. Domine and P. Tsang, https://arxiv.org/abs/1903.05663
- General algorithm for point cloud clustering → applications to water Cherenkov detectors.
- Future directions involve improving post-processing time complexity and addressing deficiencies for track clustering.

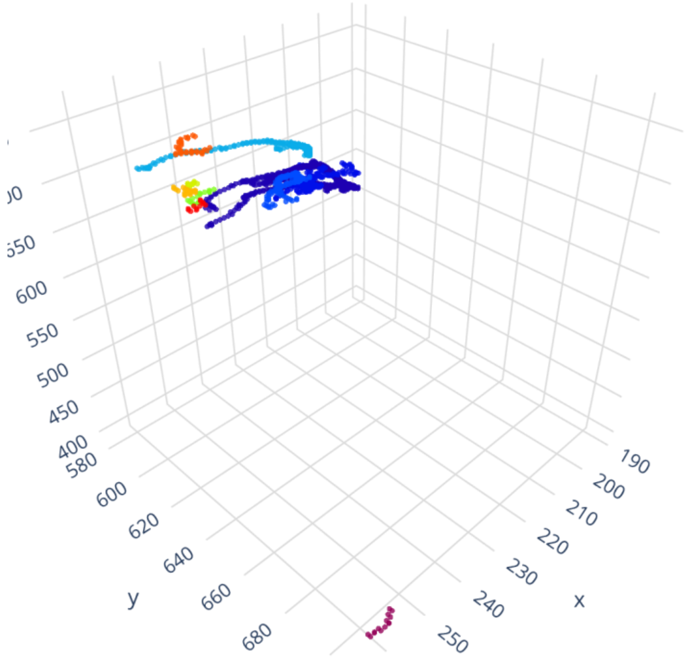
[1]: https://github.com/DeepLearnPhysics/lartpc_mlreco3d

A. Shower Mistakes

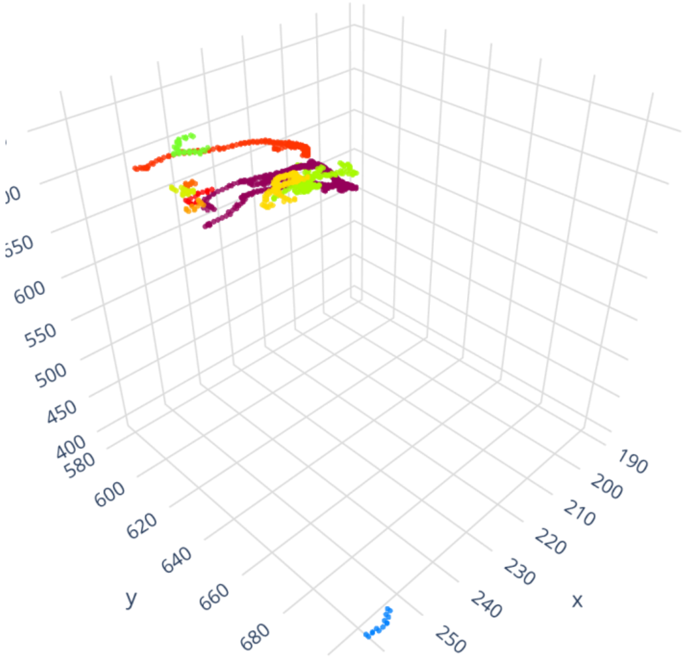
Prediction, ARI = 0.1576

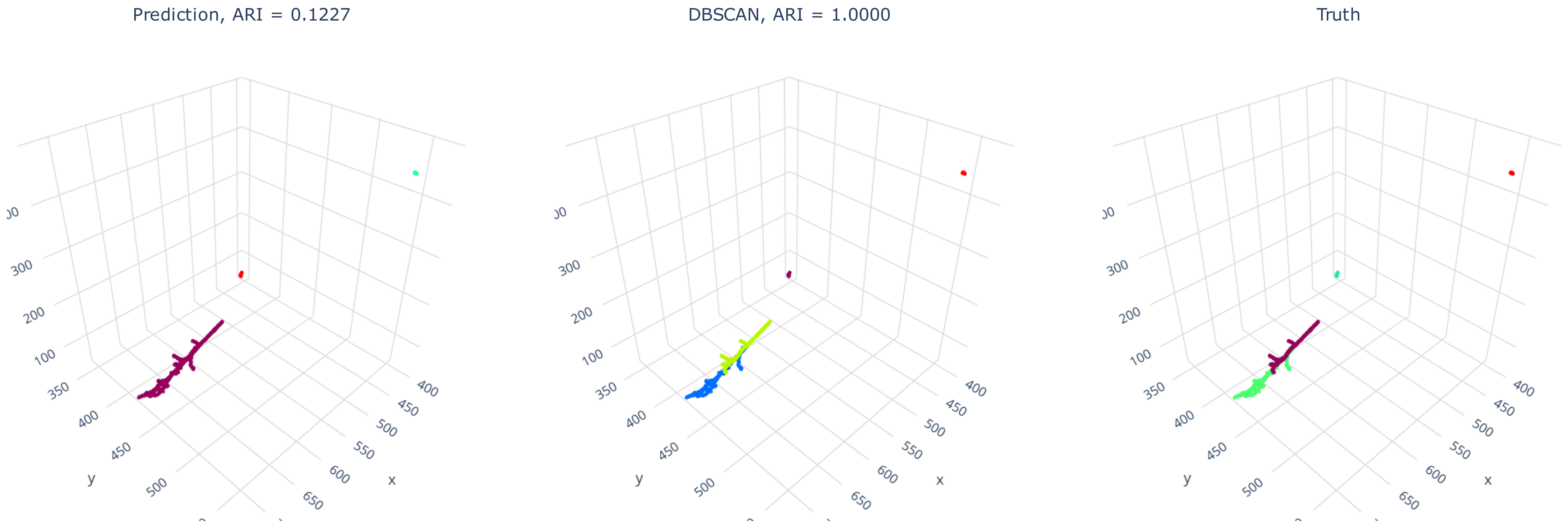


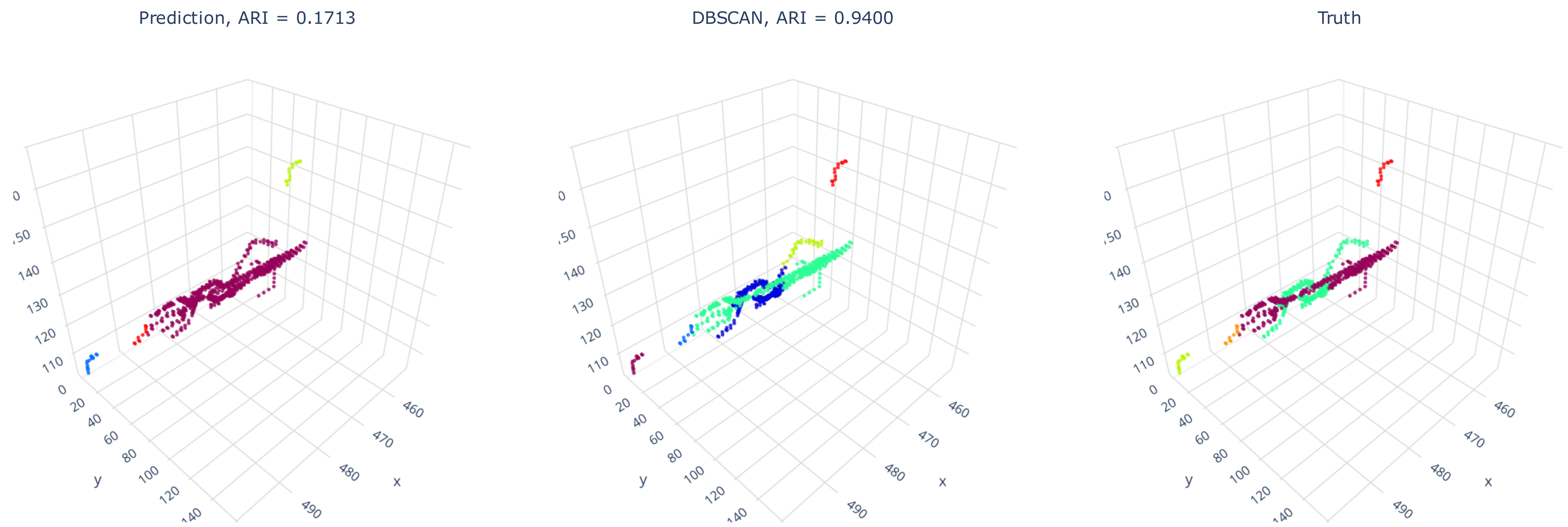
DBSCAN, ARI = 0.9994



Truth

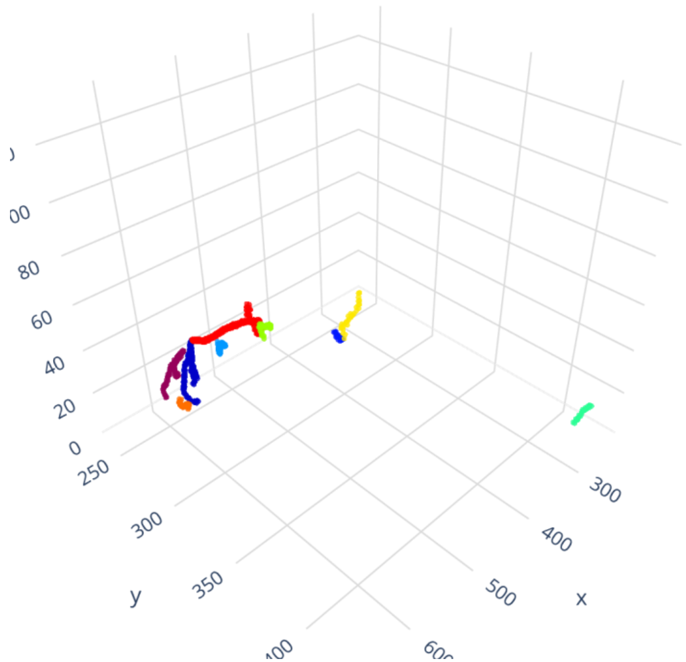



Prediction, ARI = 0.1227
DBSCAN, ARI = 1.0000
Truth
300
200
100
350
400
450
500
y
400
450
500
550
600
650
x

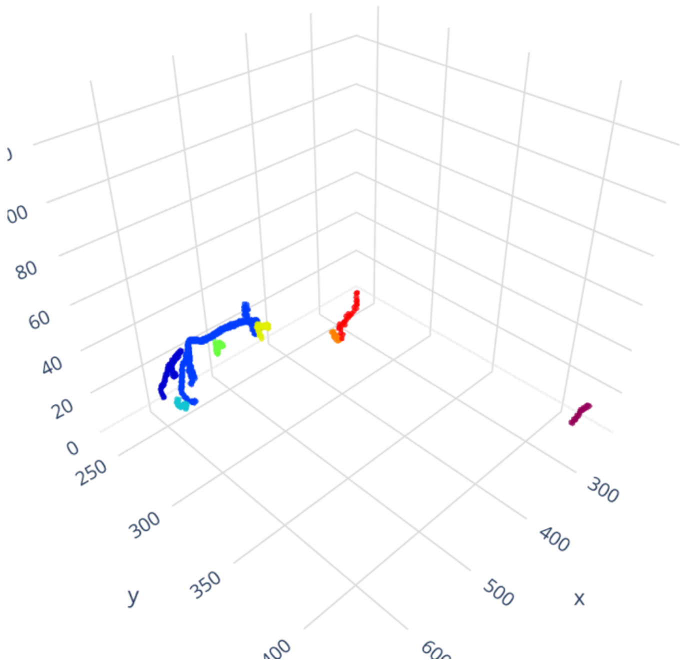

Prediction, ARI = 0.1713
DBSCAN, ARI = 0.9400
Truth
x
y
460
470
480
490
0
20
40
60
80
100
120
110
120
130
140

B. Why not DBSCAN?

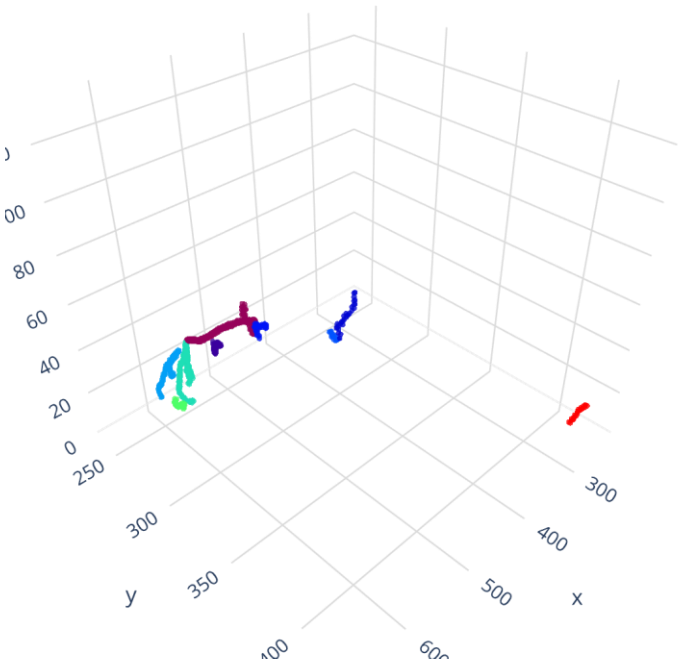
Prediction, ARI = 0.9946



DBSCAN, ARI = 0.6057



Truth



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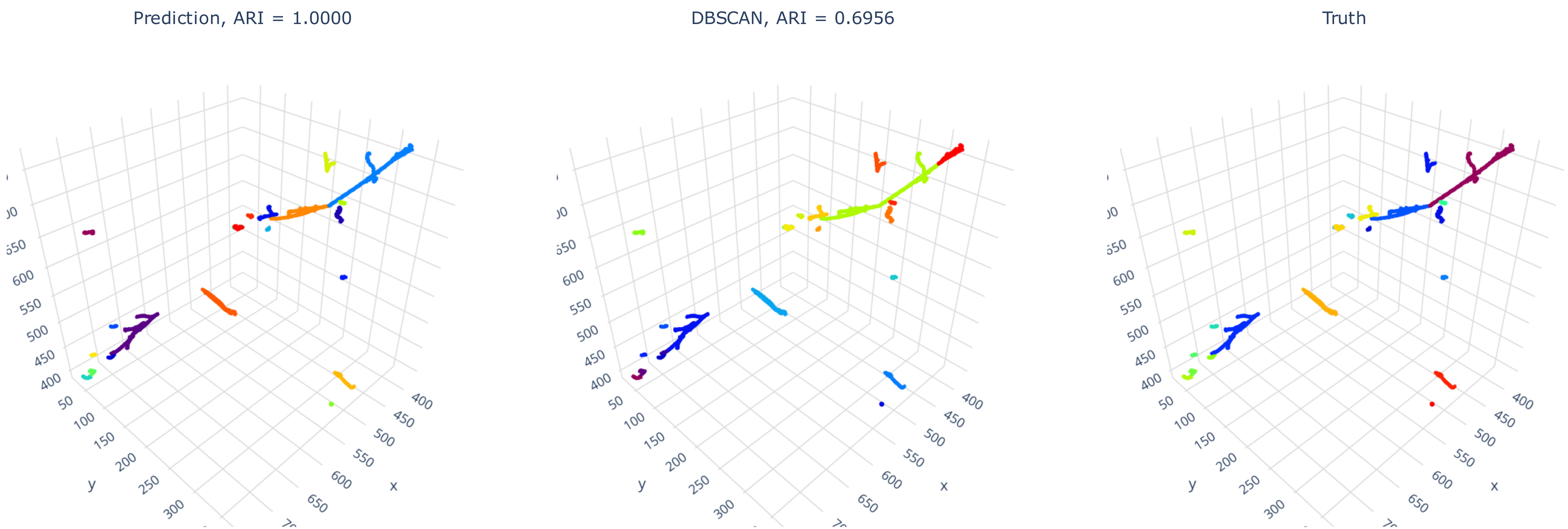
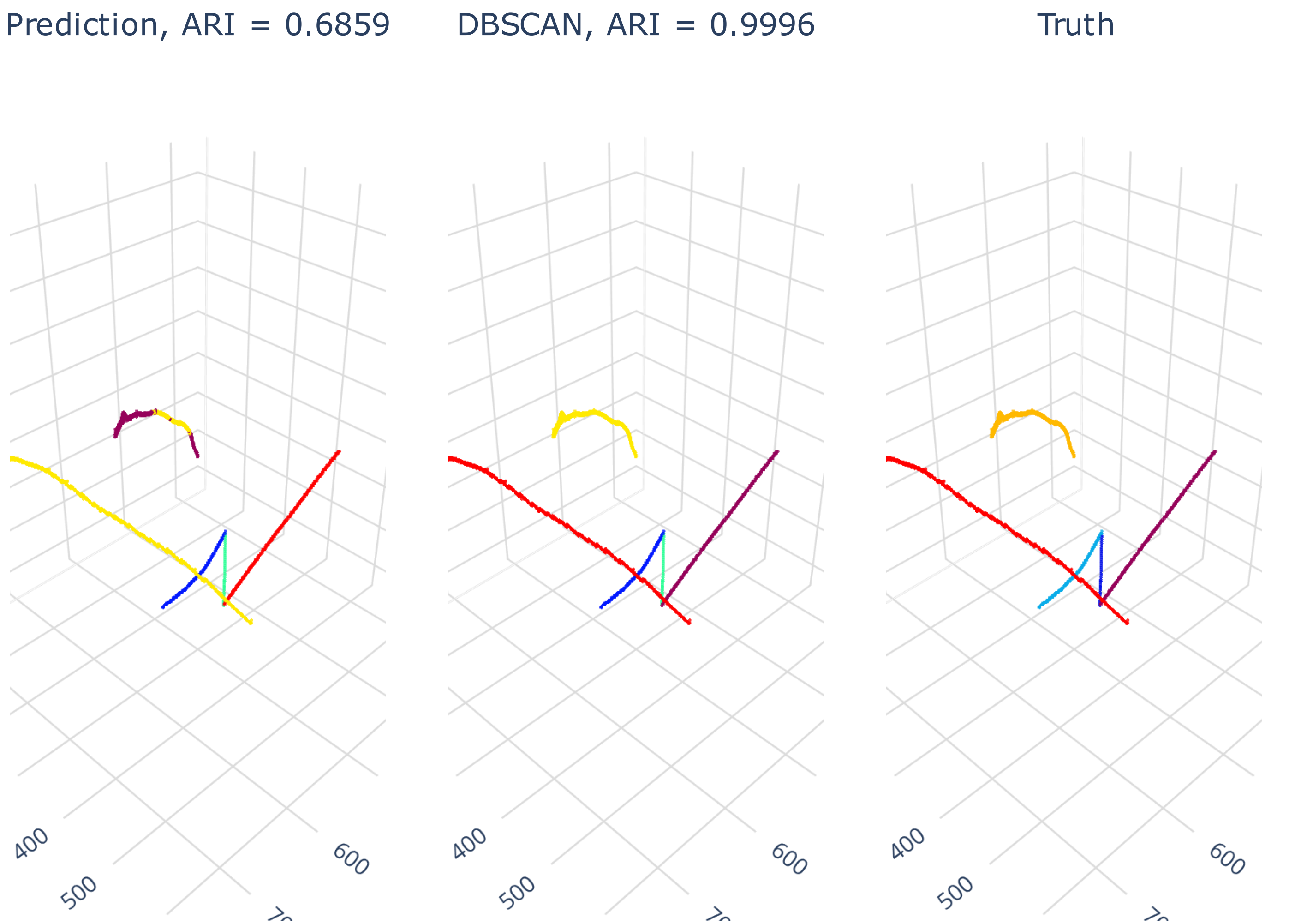
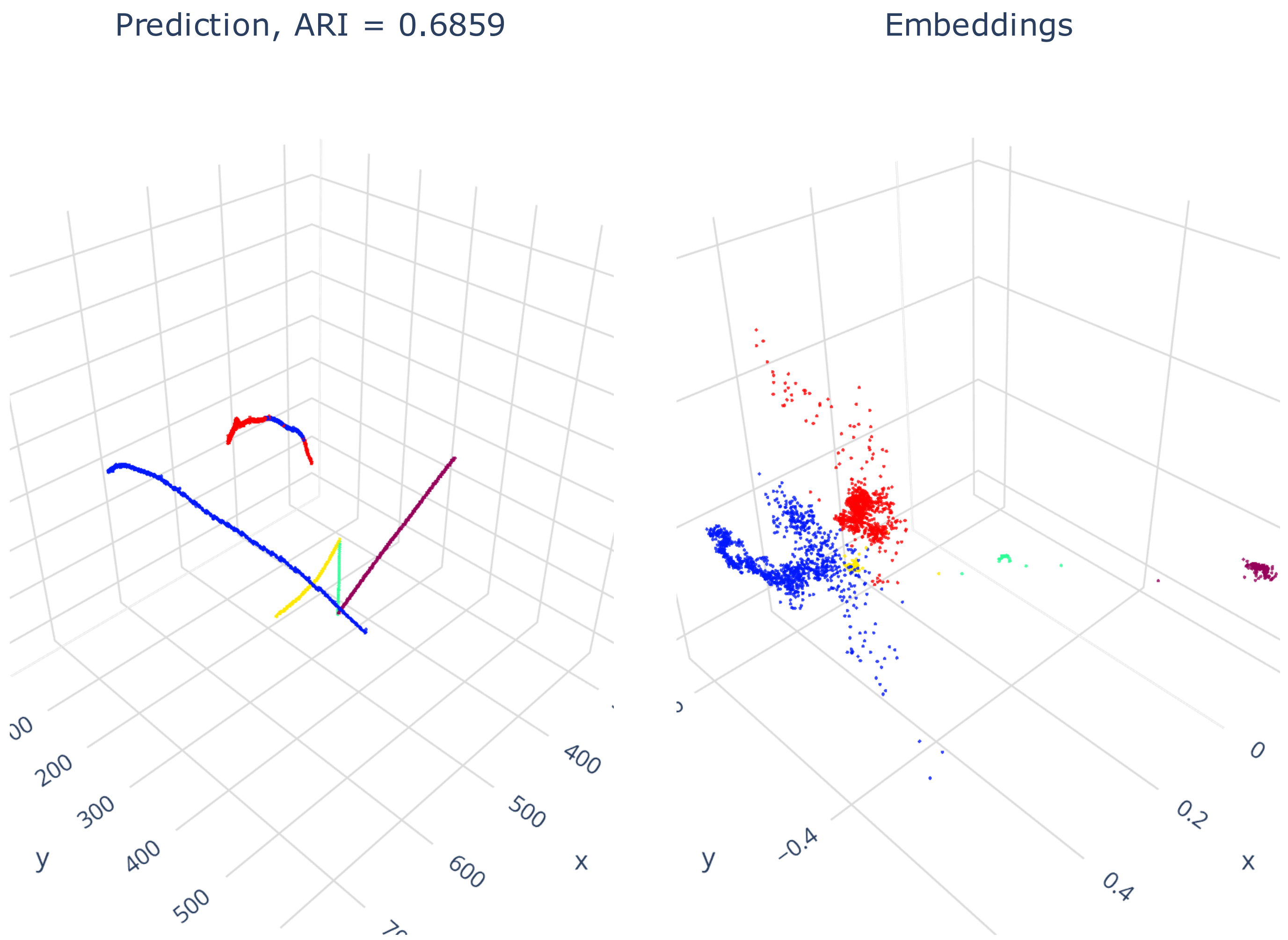
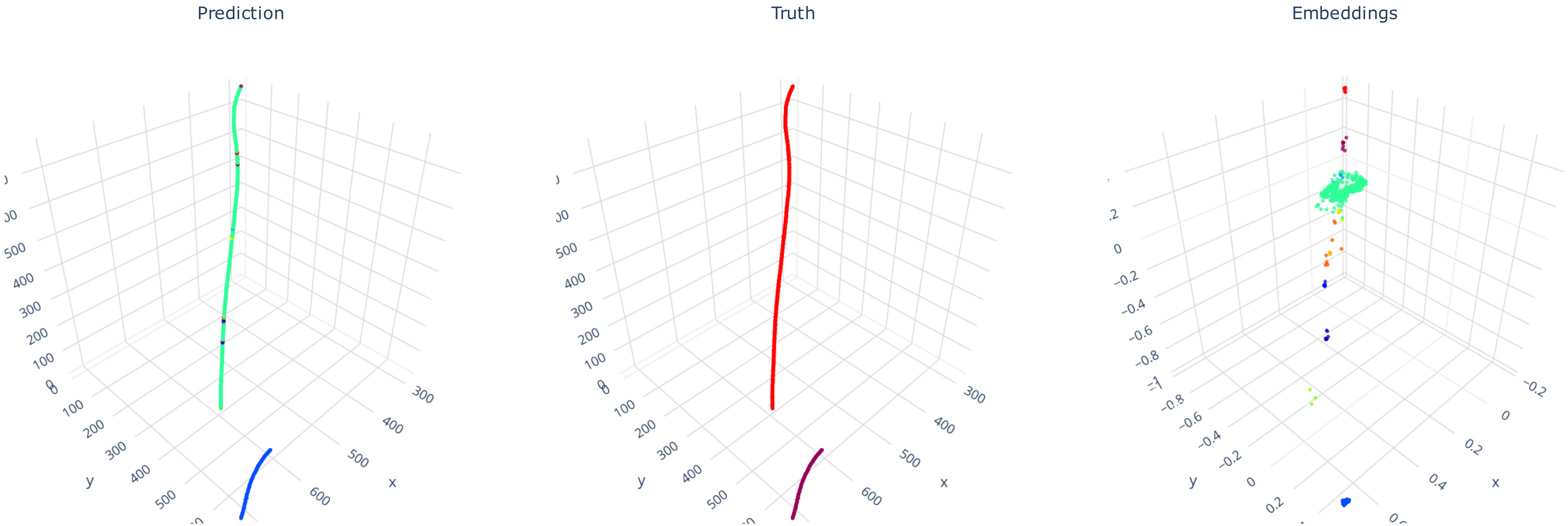


C. Track Mistakes



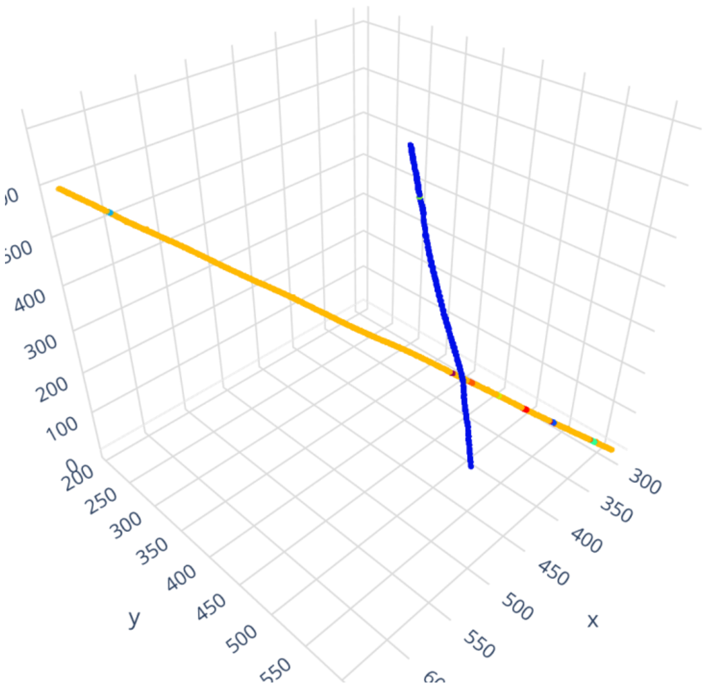

Prediction, ARI = 0.6859
Embeddings
y
x
200
300
400
500
400
500
600
y
x
−0.4
0
0.2
0.4

D. High ARI but Low SBD

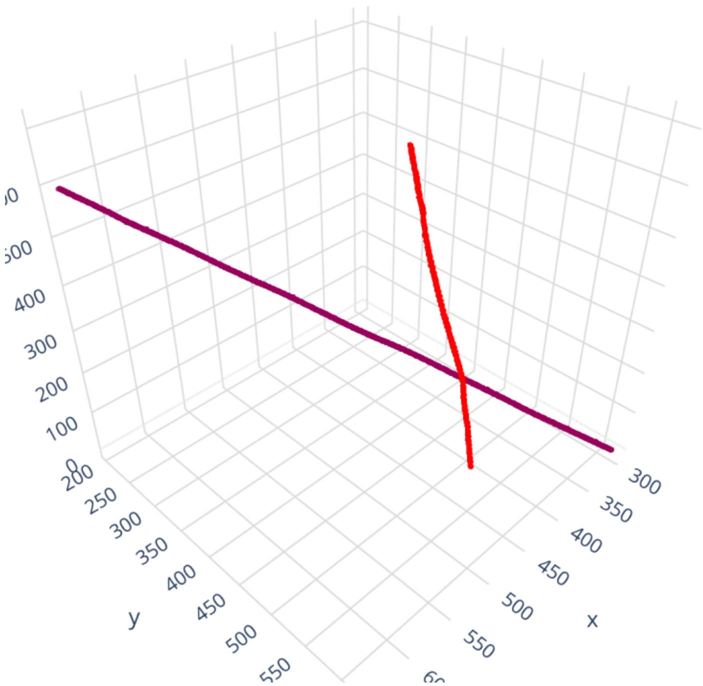


D. High ARI but Low SBD

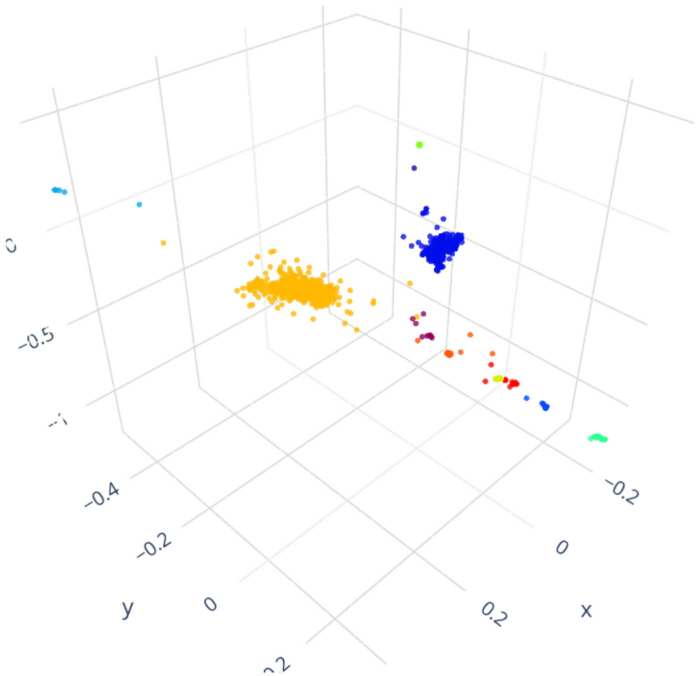
Prediction



Truth

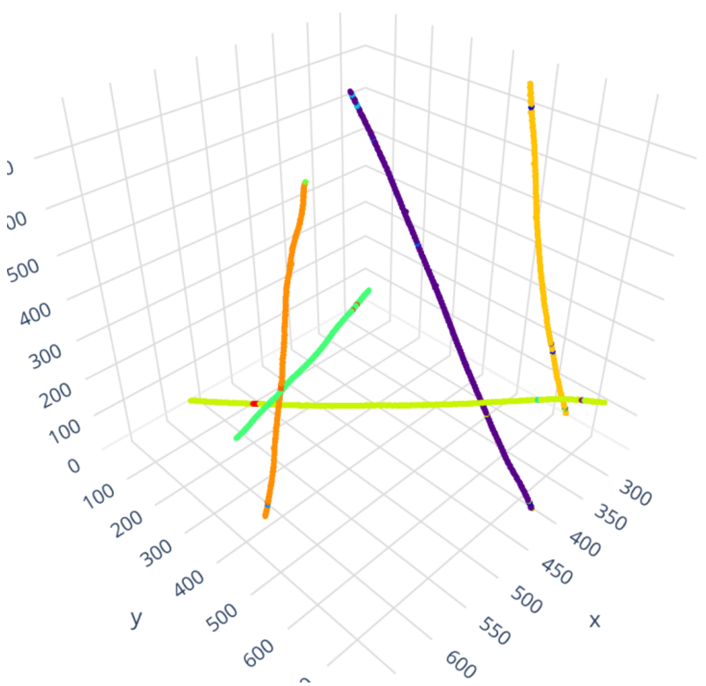


Embeddings

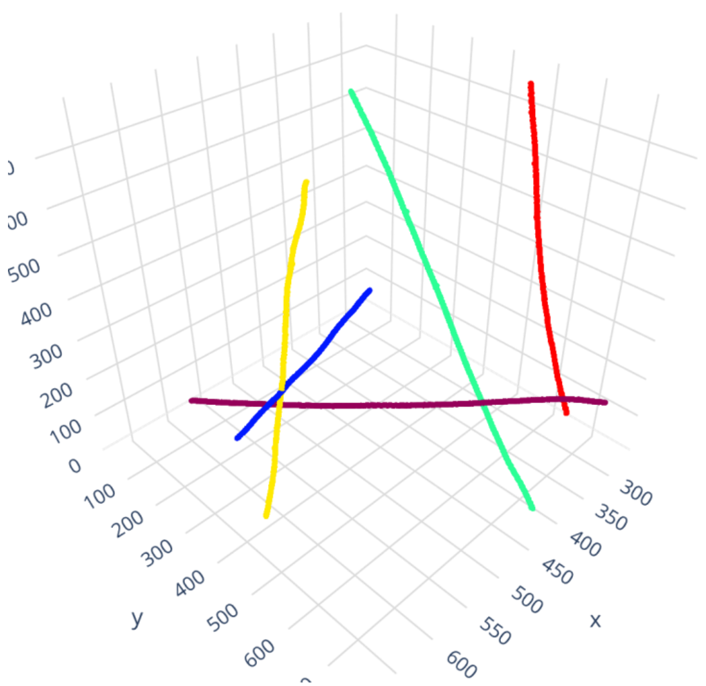


D. High ARI but Low SBD

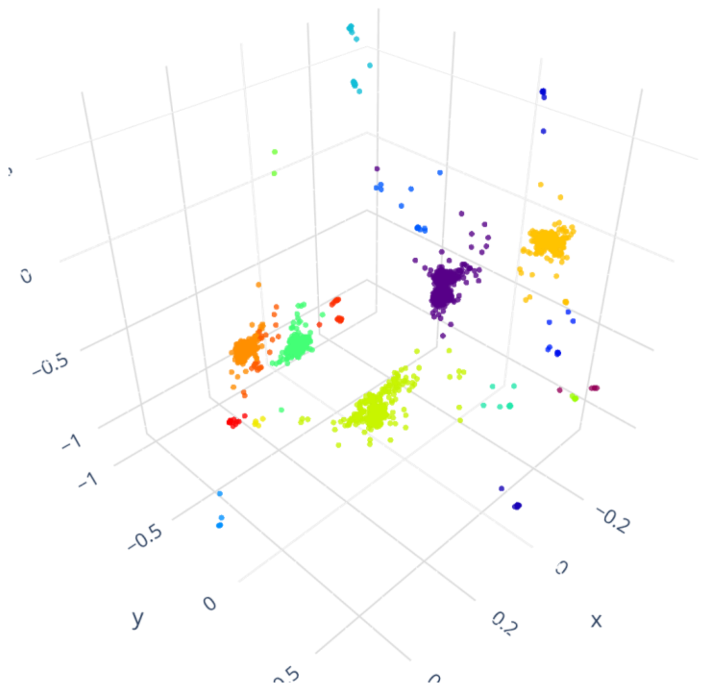
Prediction



Truth



Embeddings



E. Accuracy Metric Definitions

Definition (Purity/Efficiency for general partitions): Let $Y^* = \{S_1^*, S_2^*, \dots, S_n^*\}$ denote the ground truth partitioning of a set of points Ω, and let $\tilde{Y} = \{\widetilde{S_1}, \widetilde{S_2}, \dots, \widetilde{S_m}\}$ be the predicted partitioning of Ω. Let c_{ij} denote the entries of the contingency matrix formed by Y^* and $\tilde{Y}$. The **purity** $P(\tilde{Y}, Y^*)$ of a predicted clustering $\tilde{Y}$ with respect to ground truth Y^* is given as

$$P(\tilde{Y}, Y^*) = \frac{1}{m} \sum_{j=1}^{m} \frac{\max_{i=1,\dots,n} c_{ij}}{|\tilde{S}_j|}$$

- Purity: for a given predicted cluster of points, find the ground truth cluster with maximum pixel overlap.

Likewise, the **efficiency** $E(\tilde{Y}, Y^*)$ is defined as

$$E(\tilde{Y}, Y^*) = \frac{1}{n} \sum_{i=1}^{n} \frac{\max_{j=1,\dots,m} c_{ij}}{|S_i^*|}$$

- Efficiency: for a given ground truth cluster of points, find the predicted cluster with maximum pixel overlap.

Definition (Dice Score): Given two sets A and B, the **Dice Coefficient** is given as:

$$DSC(A,B) = \frac{2|A \cap B|}{|A| + |B|}.$$

For general partitions $Y^* = \{S_1^*, S_2^*, \dots, S_n^*\}$ and $\tilde{Y} = \{\widetilde{S_1}, \widetilde{S_2}, \dots, \widetilde{S_m}\}$, we define the **Best Dice** score of truth labels Y^* with respect to predictions $\tilde{Y}$:

$$BD(Y^*, \tilde{Y}) = \frac{1}{n} \max_{j=1,\dots,m} DSC(S_i^*, \widetilde{S_j}).$$

After symmetrizing, we obtain the **Symmetric Best Dice** score:

$$SBD(Y^*, \tilde{Y}) = \min\{BD(Y^*, \tilde{Y}), BD(\tilde{Y}, Y^*)\}.$$