WP12: Software for Future Detectors

Frank Gaede (DESY) and Graeme Stewart (CERN), for the WP12 team

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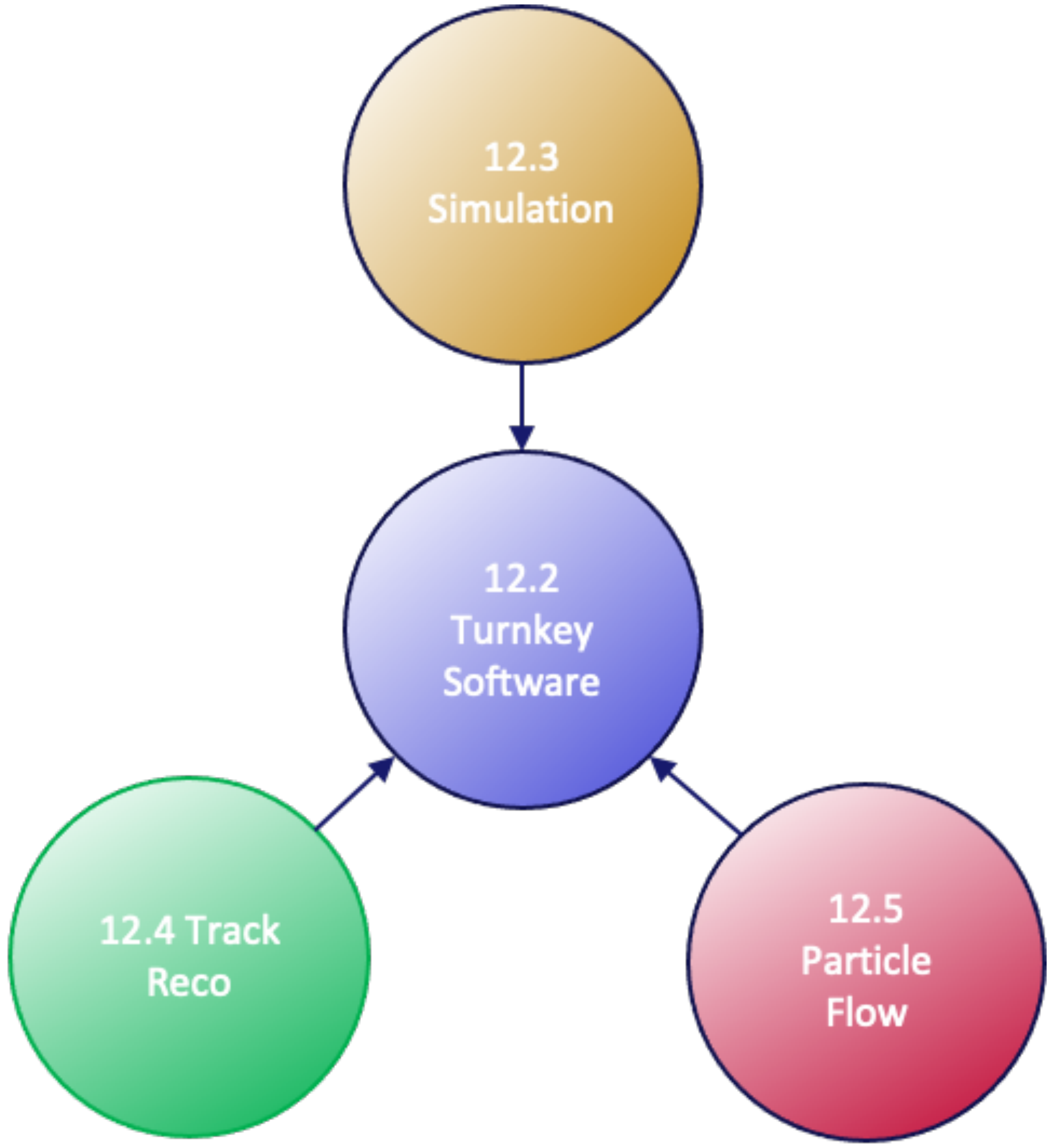
AIDAinnova 3rd Annual Meeting, Catania
2024-03-21

Tasks, Partners and Task Leaders in WP12

- Task 12.1. Coordination and Communication **(CERN, DESY)**
  - Graeme Stewart, Frank Gaede
- Task 12.2. Turnkey Software **(DESY, CERN, INFN-PI, INFN-PD, INFN-BA, INFN-BO,** IHEP, SDU**)**
  - Turnkey Software Stack, for physics and performance studies, EDM4hep, PODIO and Digitisation toolkit
  - R&D study on frameworks to manage heterogeneous resources
  - Thomas Madlener, André Sailer
- Task 12.3. Simulation **(CERN, DESY, CNRS-IJCLab, UNIMAN)**
  - Fast simulation techniques integrated into Geant4
  - Machine learning based calorimeter simulation toolkit for training and inference
  - Anna Zaborowska
- Task 12.4. Track Reconstruction **(CNRS-IJCLab, CERN, DESY, INFN-FE, INFN-BO)**
  - complete track reconstruction with ACTS composable algorithms and for heterogeneous computing
  - Machine learning reconstruction algorithm for MPGD detectors
  - Hadrien Grasland
- Task 12.5. Particle Flow Reconstruction **(UWAR, CERN, INFN-RM3, CNRS-LLR, CNRS-IP2I, UOS)**
  - PFA algorithms for DUNE and dual-readout calorimeters, APRIL PFA for hadronic jets
  - John Back, John Marshal



Milestones ✅ and Deliverables 📆

in WP12

Milestone	Title	Due Date
MS48	LC reconstruction prototype in Key4hep	M21
MS49	Prototype of ML based shower simulation	M22
MS50	ACTS tracking algorithm prototypes	M23
MS51	New PFA prototypes	M23

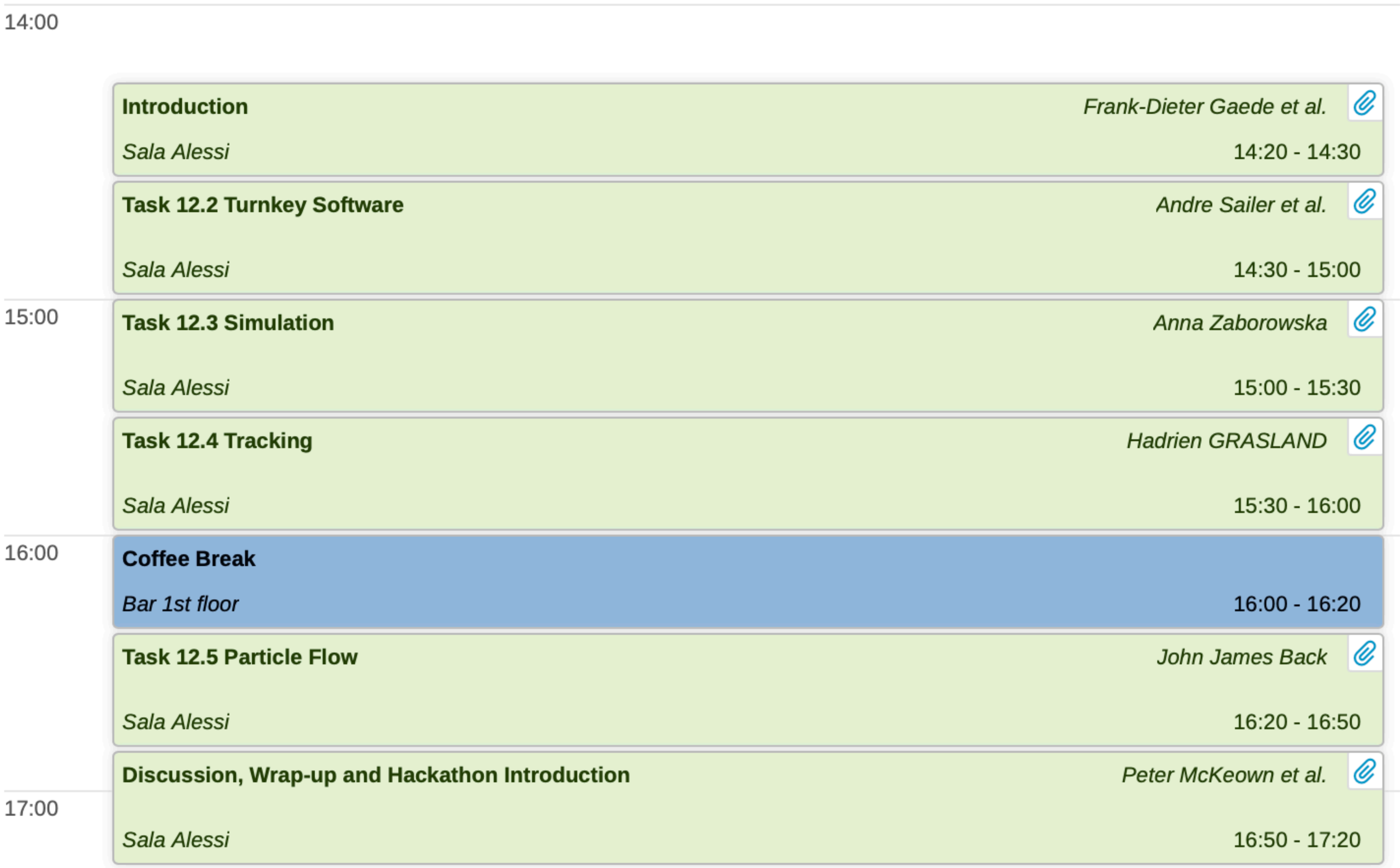
All milestones were achieved on time ✓

Substantial progress in all tasks, currently no significant concerns for meeting these deliverables on time

Deliverable	Title		Due Date
D12.1	Turnkey Software Stack (Key4hep)	**Fully functional turnkey software stack** (Key4hep) with **simulation**, **track reconstruction** and **particle flow** algorithms running for the **linear colliders and the FCC**, using the common event data model (EDM4hep), with **documentation and examples**	M46 (Jan 25)
D12.2	Fast shower simulation in Geant4	**Fast shower simulation** based on **parameterisations** and based on **machine learning** techniques fully integrated in Geant4, released with **documentation and examples**	M45 (Dec 24)
D12.3	ACTS tracking algorithms	**Track reconstruction algorithms** incorporated into ACTS, and **fully documented**, that manage the full tracking chain **on CPU and non-CPU devices**, with optional machine learning based algorithms available, also supporting MPGD detectors	M43 (Oct 24)
D12.4	PFA reconstruction	**Improved and documented particle flow algorithms**, including **machine learning based algorithms**, available in the **PandoraPFA toolkit**, suitable for detectors using new readout technology	M45 (Dec 24)

WP12 in Catania

- WP12 session ran on Monday afternoon
- We also took advantage of being here in Catania and ran a *hackathon*



14:00

Introduction — *Frank-Dieter Gaede et al.*
Sala Alessi — 14:20 - 14:30

Task 12.2 Turnkey Software — *Andre Sailer et al.*
Sala Alessi — 14:30 - 15:00

15:00

Task 12.3 Simulation — *Anna Zaborowska*
Sala Alessi — 15:00 - 15:30

Task 12.4 Tracking — *Hadrien GRASLAND*
Sala Alessi — 15:30 - 16:00

16:00

Coffee Break
Bar 1st floor — 16:00 - 16:20

Task 12.5 Particle Flow — *John James Back*
Sala Alessi — 16:20 - 16:50

Discussion, Wrap-up and Hackathon Introduction — *Peter McKeown et al.*

17:00

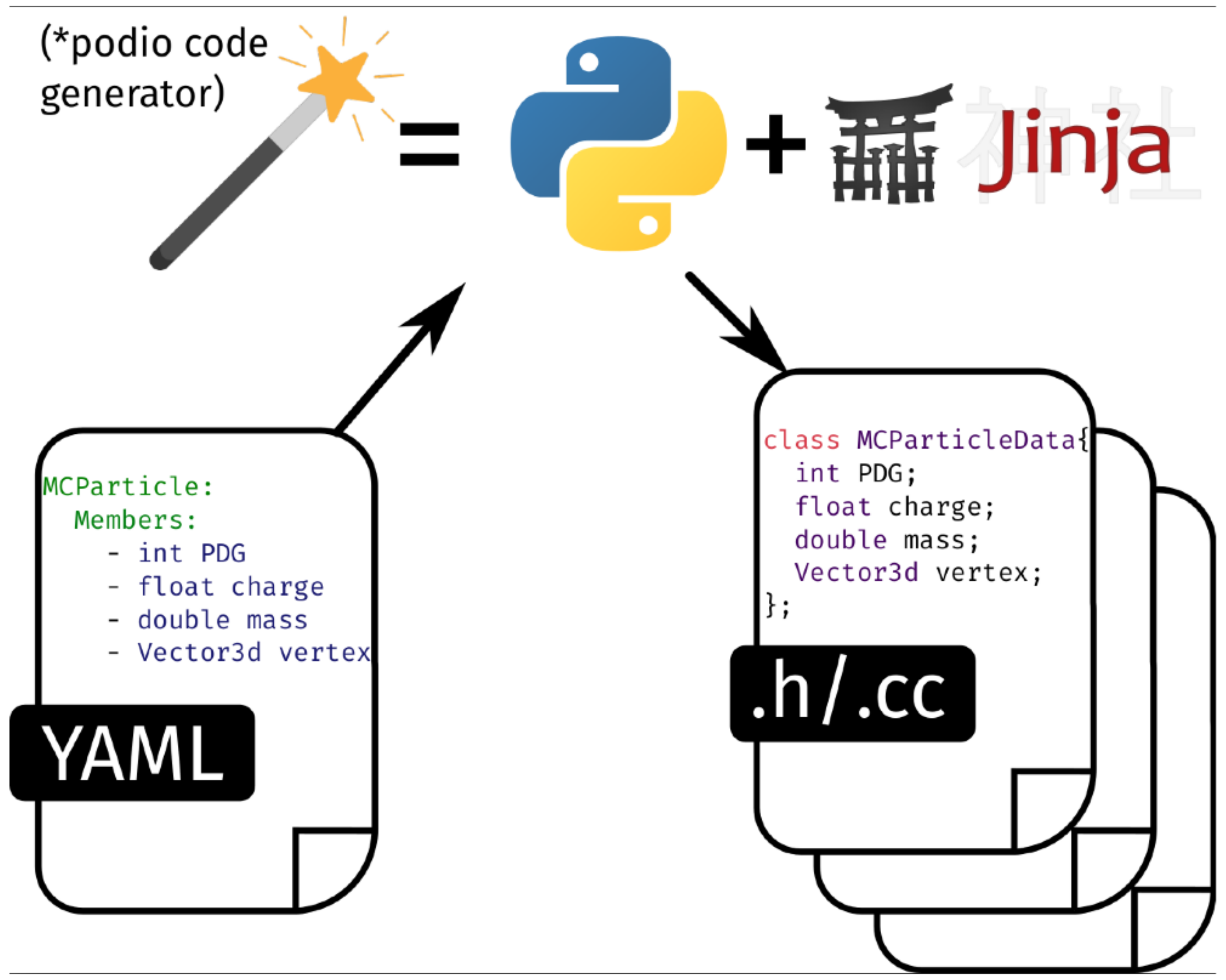
Sala Alessi — 16:50 - 17:20

Turnkey Software

Turnkey Stack: PODIO

Event data model toolkit using *Plain Old Data IO*

- Driven by a YAML description of the data model, from which PODIO generates code

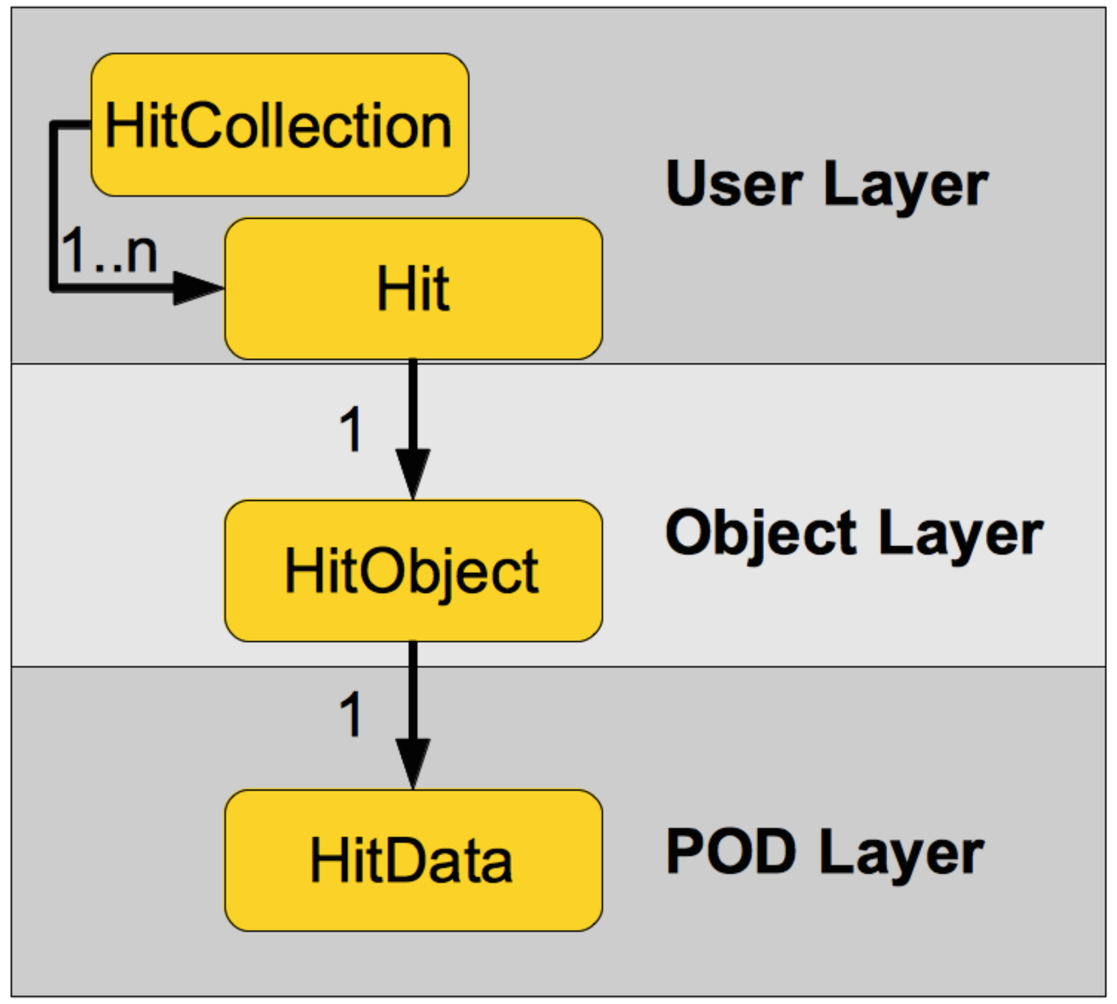


```
MCParticle:
  Members:
    - int PDG
    - float charge
    - double mass
    - Vector3d vertex
```

```
class MCParticleData{
  int PDG;
  float charge;
  double mass;
  Vector3d vertex;
};
```

- Major items delivered this year

✅ **Schema evolution** of generated EDMs (basic use cases, extend as necessary)
✅ RNTuple based backend (new ROOT storage backend)
✅ Stable collection IDs (necessary for multithreading)
✅ Interface types (inheritance free interfaces)
✅ First version of Julia code generation
✅ Completely moved to *Frame* based I/O



Turnkey Stack: EDM4hep

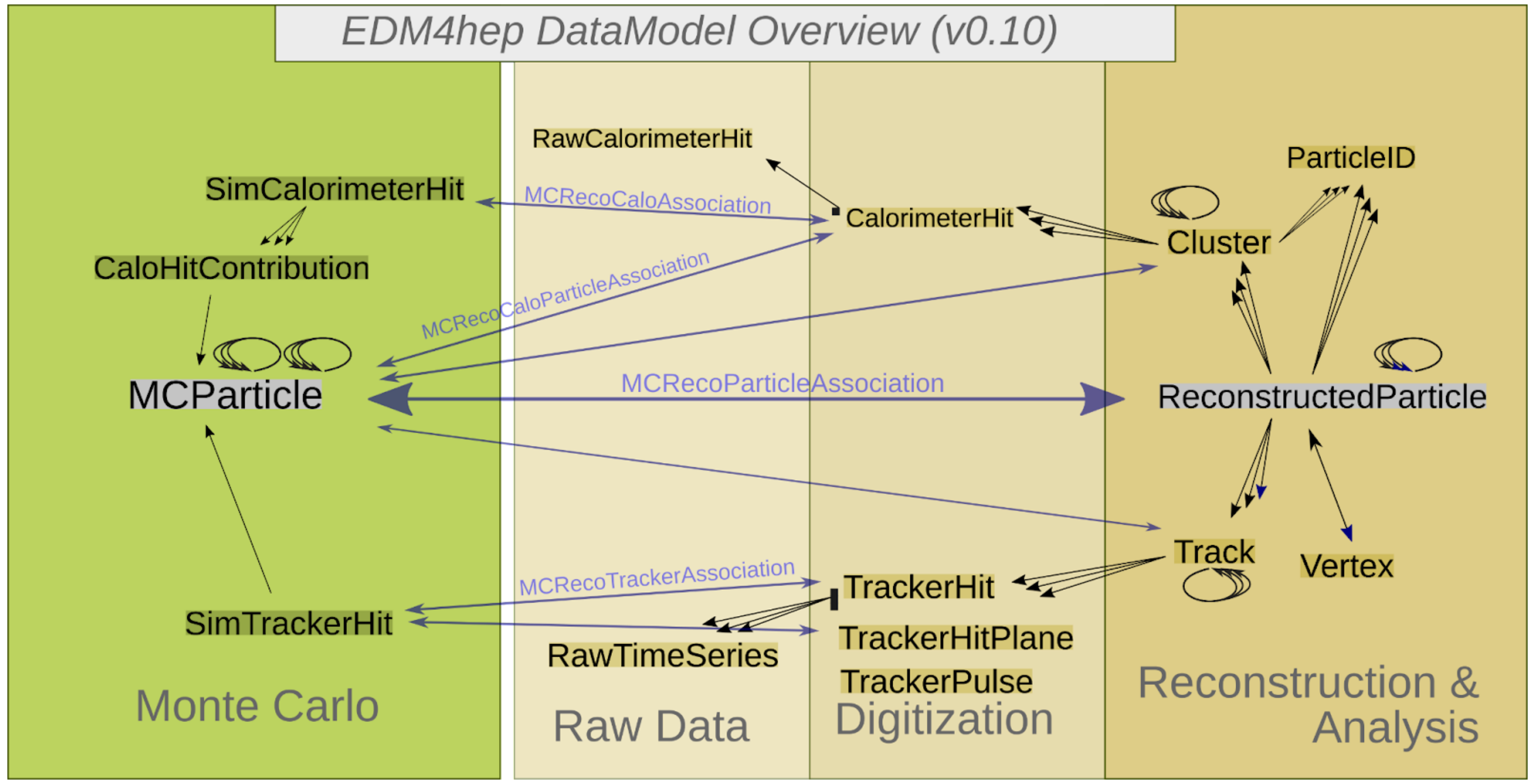
- EDM4hep defines the common language for all Key4hep components to communicate
- Generated by the PODIO EDM toolkit
- Major items from this year:

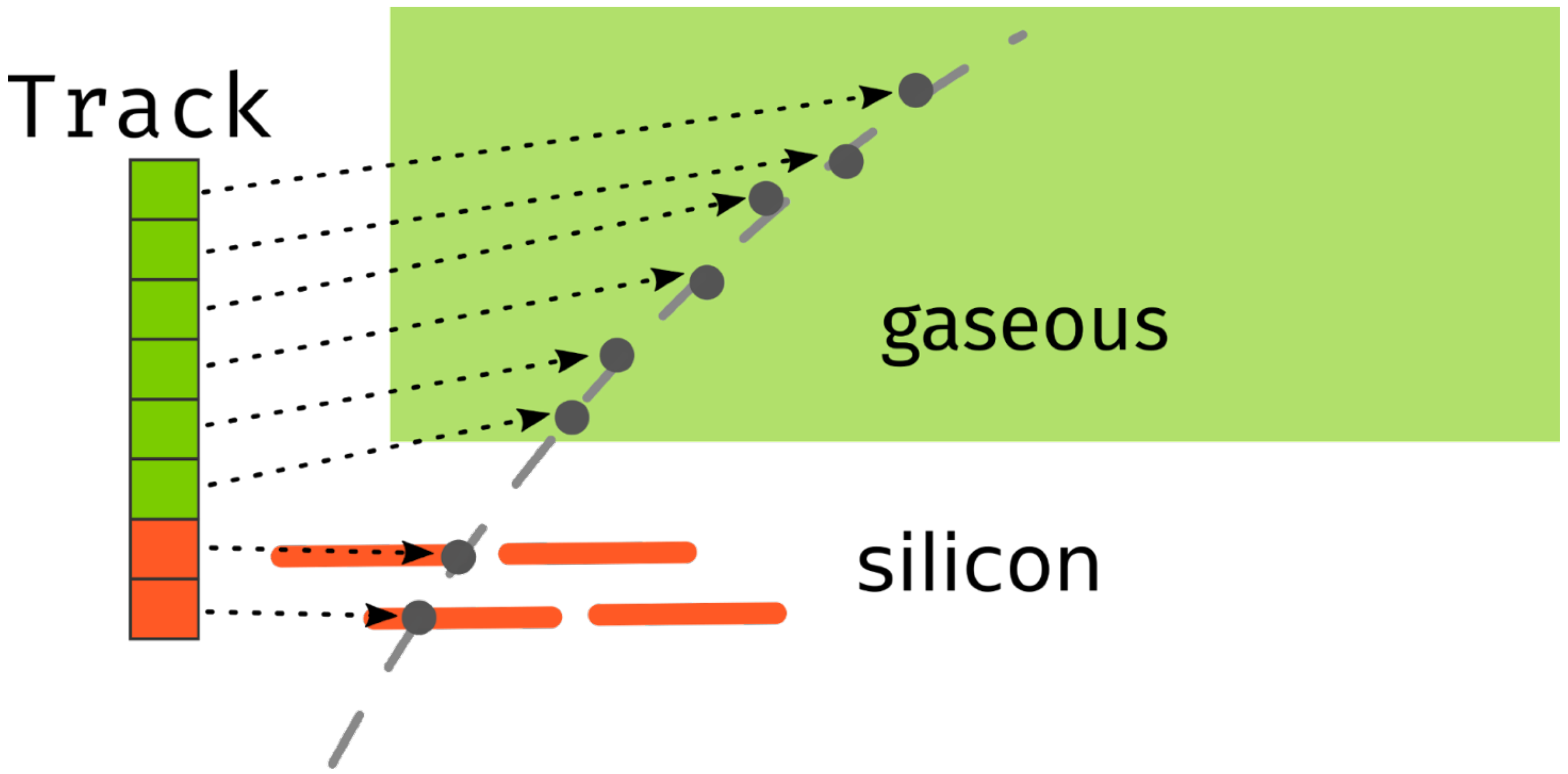
✅ (Standalone) conversion from LCIO

✅ Improved python bindings

✅ Introduction of TrackerHit interface (covering TrackerHit3D and TrackerHitPlane)

✅ Cleanup of type inconsistencies / naming / documentation

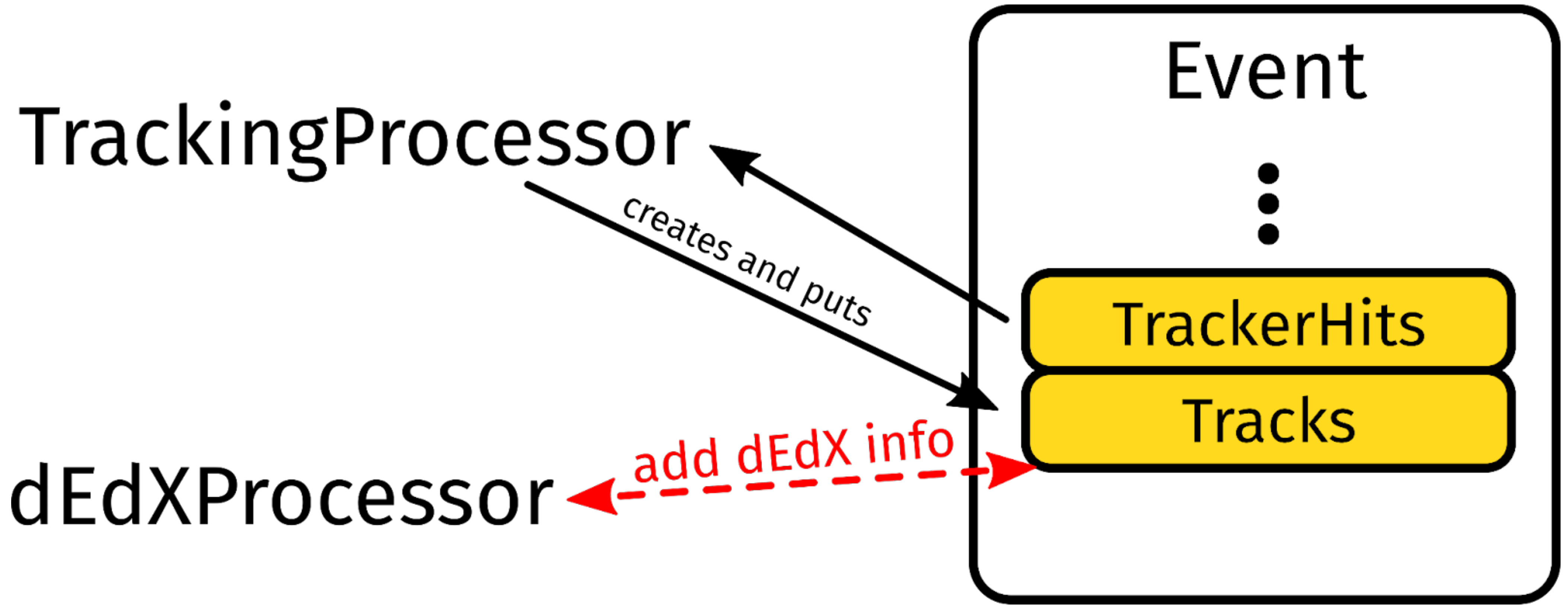


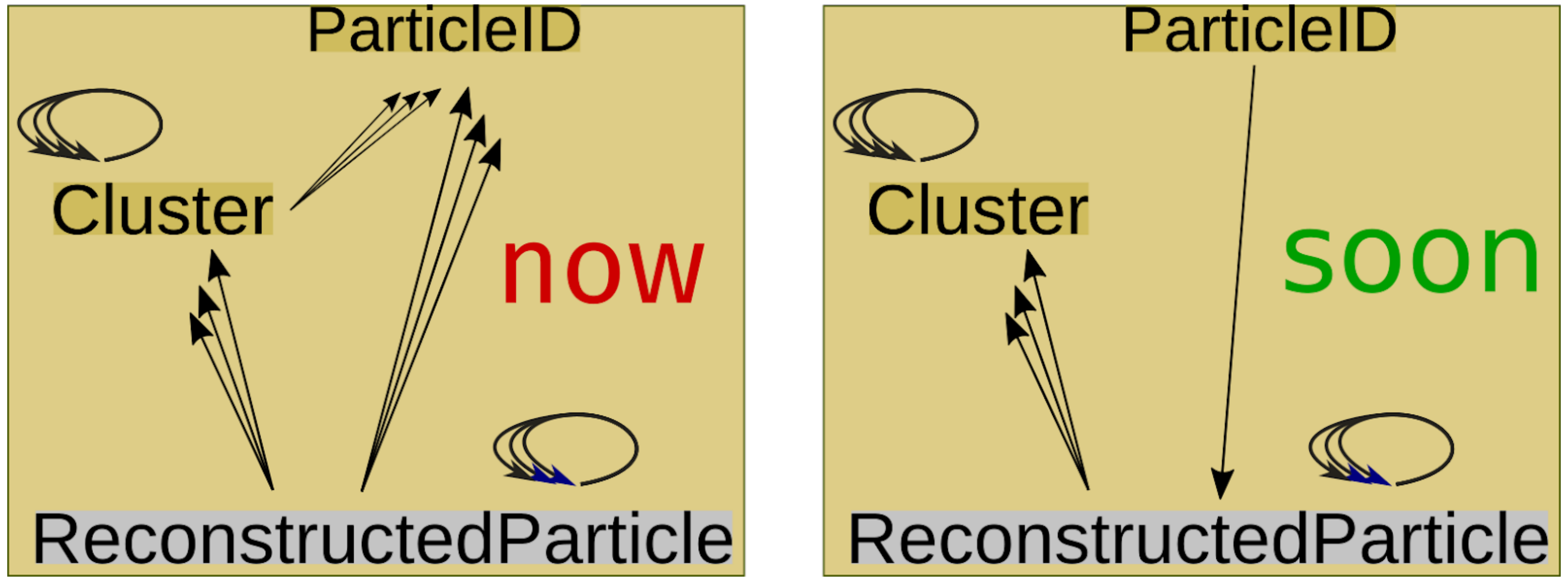


EDM4hep v1.0

The last missing pieces

- Breaking things without intention of doing schema evolution
  - Too many things that do not have an easy evolution mechanism
- **Consistent mutability concept**
  - Some inconsistencies inherited from LCIO
  - Very big conceptual change
  - Requires substantial work in conversion
  - Requires new utilities for users
- Many things already addressed
  - TrackerHit interface
  - Multiple EventWeights
  - Consistent relation naming
- Keeping track in EDM4hep v1.0 github project





Key4hep

One stack to rule them all…

- This is the full stack for future detectors based on PODIO, EDM4hep and Gaudi
- More than 500 packages built with Spack
- Releases in `/cvmfs/sw.hsf.org` with tagged versions of the packages
- Key improvements

✅ Switch FW core to use PODIO Frames (+removal of legacy EventStore)

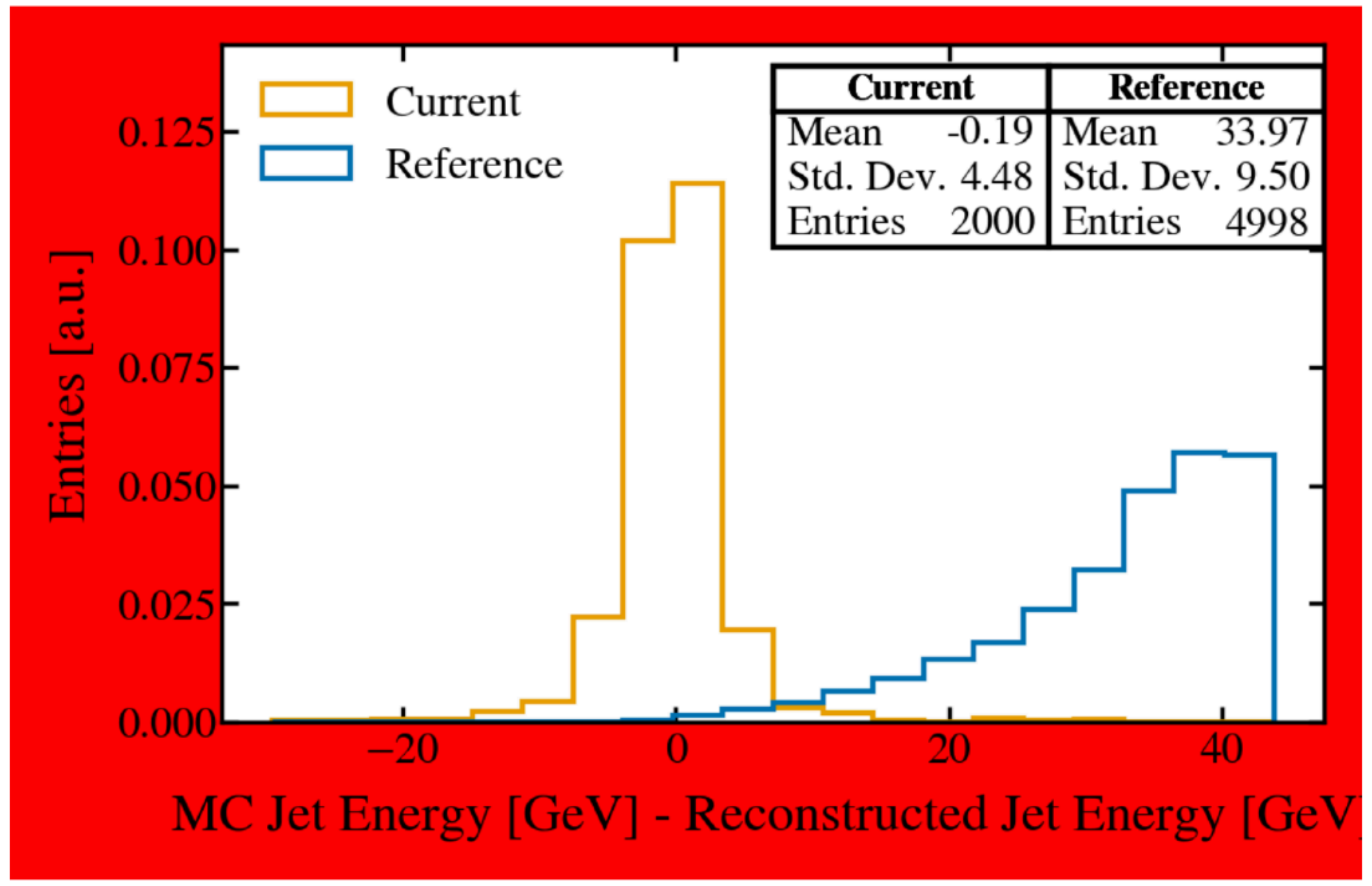
✅ Unified all EDM4hep ↔ LCIO converters in one library (k4MarlinWrapper)

✅ Thread safety metadata handling and Gaudi Functional algorithms

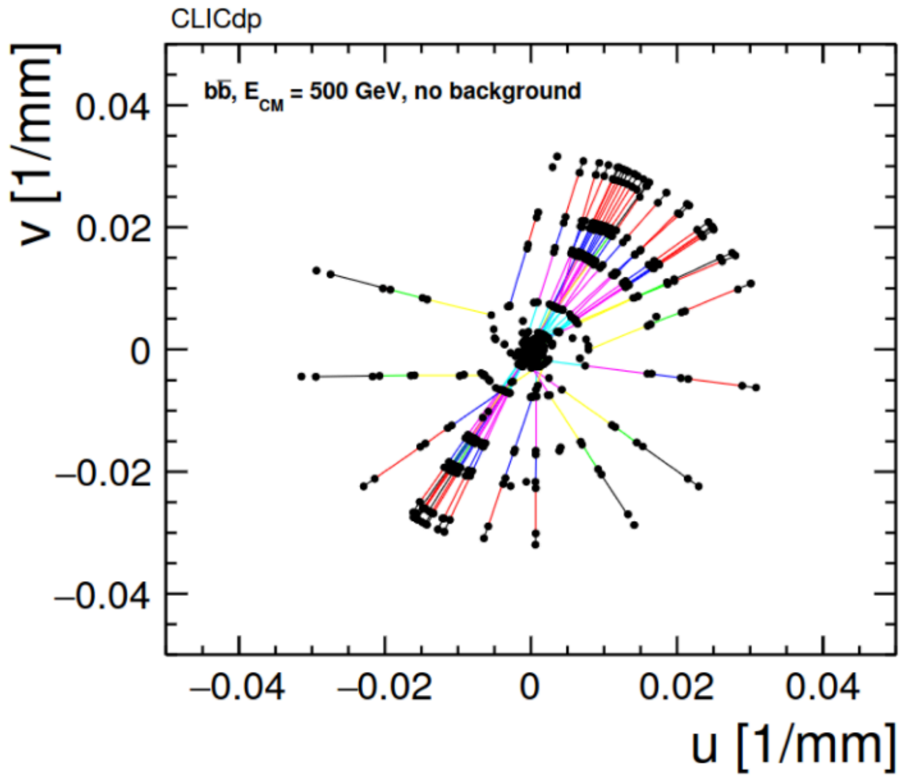
✅ Builds on AlmaLinux9 and Ubuntu 22 (and still CentOS7, but it is ~EOL)

✅ New validation system checks physics output from simulation and reconstruction: https://key4hep-validation.web.cern.ch/

👷 Progress in integration of ACTS (tracking) and PandoraPFA (particle flow)

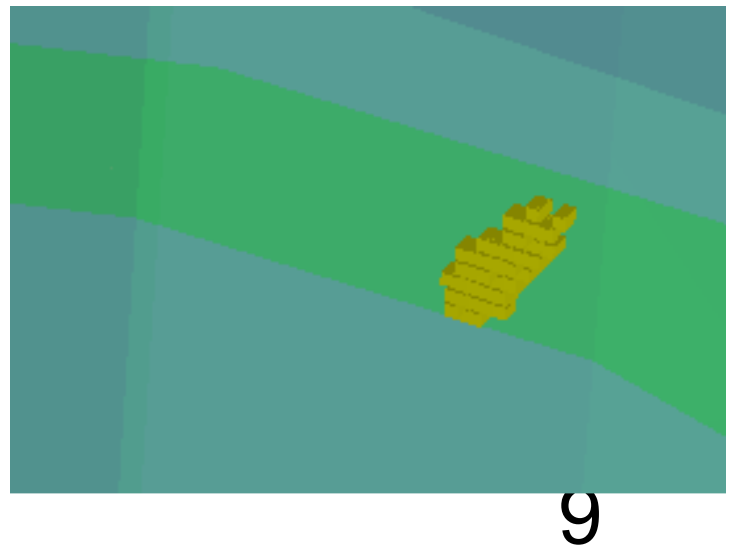


	Current	Reference
Mean	-0.19	33.97
Std. Dev.	4.48	9.50
Entries	2000	4998



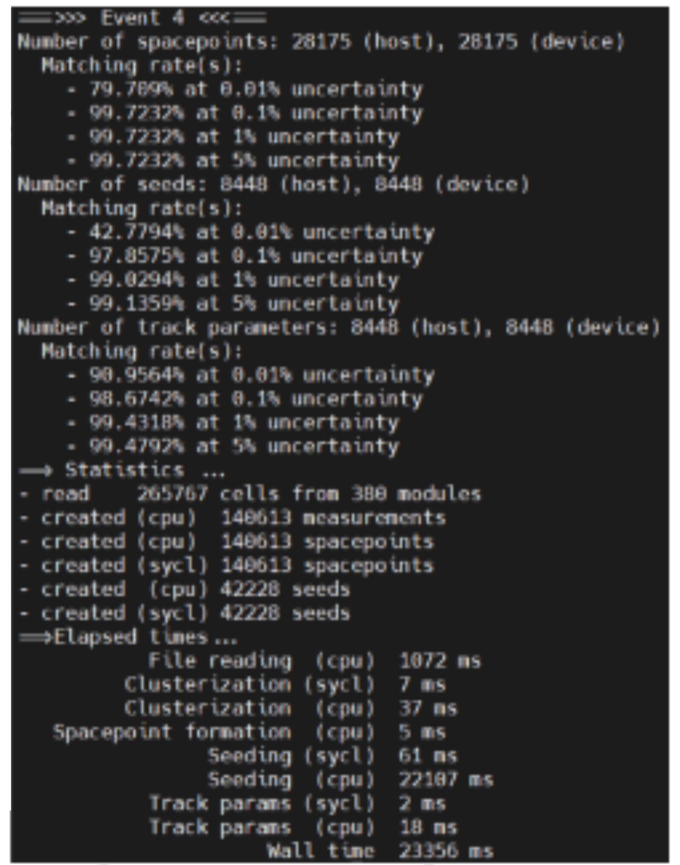
ACTS reconstructed tracks

PandoraPFA clusters in LAr FCC detector



Other Turnkey News

- INFN
  - Unable to hire for the work on managing heterogeneous resources
  - They will now redirect the funds to other areas (TBD)
- IHEP
  - Extend EDM4hep to support ongoing activities in CEPC
  - CEPC Vertex Detector tracking with ACTS
  - CEPC-on-Gaussino prototype (based on LHCb simulation infrastructure)
- SDU
  - Development of an analysis toolkit based on RDataFrame
  - Further development of Valprod toolkit to run CEPC validation

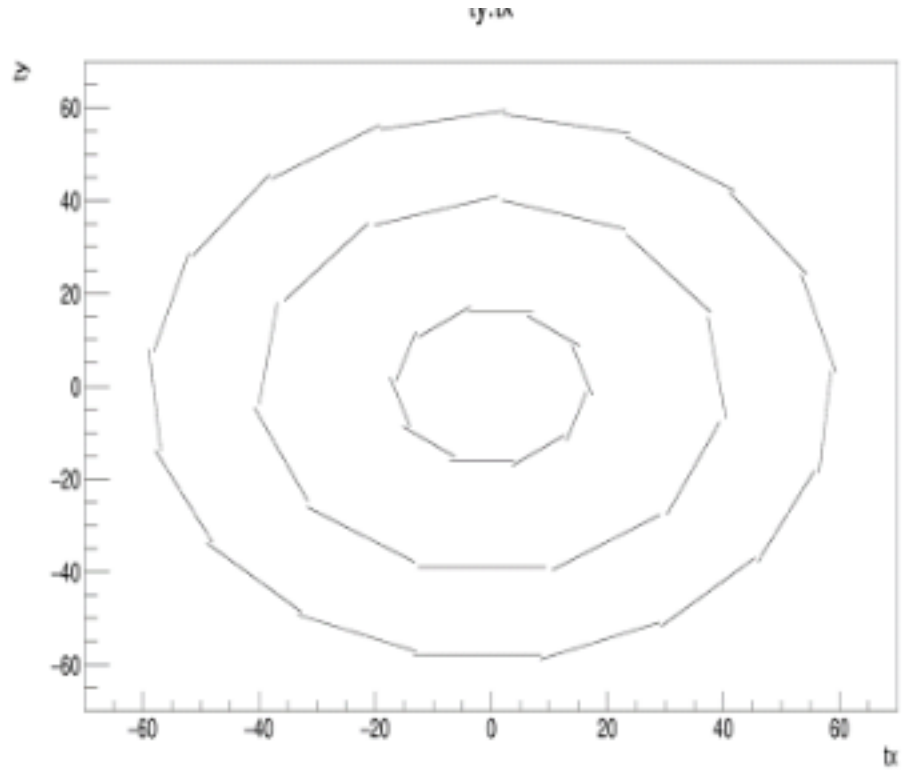


```
══>>> Event 4 <<<══
Number of spacepoints: 28175 (host), 28175 (device)
  Matching rate(s):
    - 79.789% at 0.01% uncertainty
    - 99.7232% at 0.1% uncertainty
    - 99.7232% at 1% uncertainty
    - 99.7232% at 5% uncertainty
Number of seeds: 8448 (host), 8448 (device)
  Matching rate(s):
    - 42.7794% at 0.01% uncertainty
    - 97.8575% at 0.1% uncertainty
    - 99.0294% at 1% uncertainty
    - 99.1359% at 5% uncertainty
Number of track parameters: 8448 (host), 8448 (device)
  Matching rate(s):
    - 98.9564% at 0.01% uncertainty
    - 98.6742% at 0.1% uncertainty
    - 99.4318% at 1% uncertainty
    - 99.4792% at 5% uncertainty
──> Statistics ...
- read    265767 cells from 388 modules
- created (cpu)  140613 measurements
- created (cpu)  140613 spacepoints
- created (sycl) 140613 spacepoints
- created  (cpu) 42228 seeds
- created (sycl) 42228 seeds
══>Elapsed times...
           File reading  (cpu)  1072 ms
         Clusterization (sycl)  7 ms
         Clusterization  (cpu)  37 ms
   Spacepoint formation  (cpu)  5 ms
                Seeding (sycl)  61 ms
                Seeding  (cpu)  22107 ms
           Track params (sycl)  2 ms
           Track params  (cpu)  18 ms
                  Wall time  23356 ms
```

Computing performance of TRACCC

CPU: Intel Xeon Silver 4214 @ 2.20GHz

GPU: NVIDIA Quadro RTX 8000



Visualization of vertex detector (single sided)

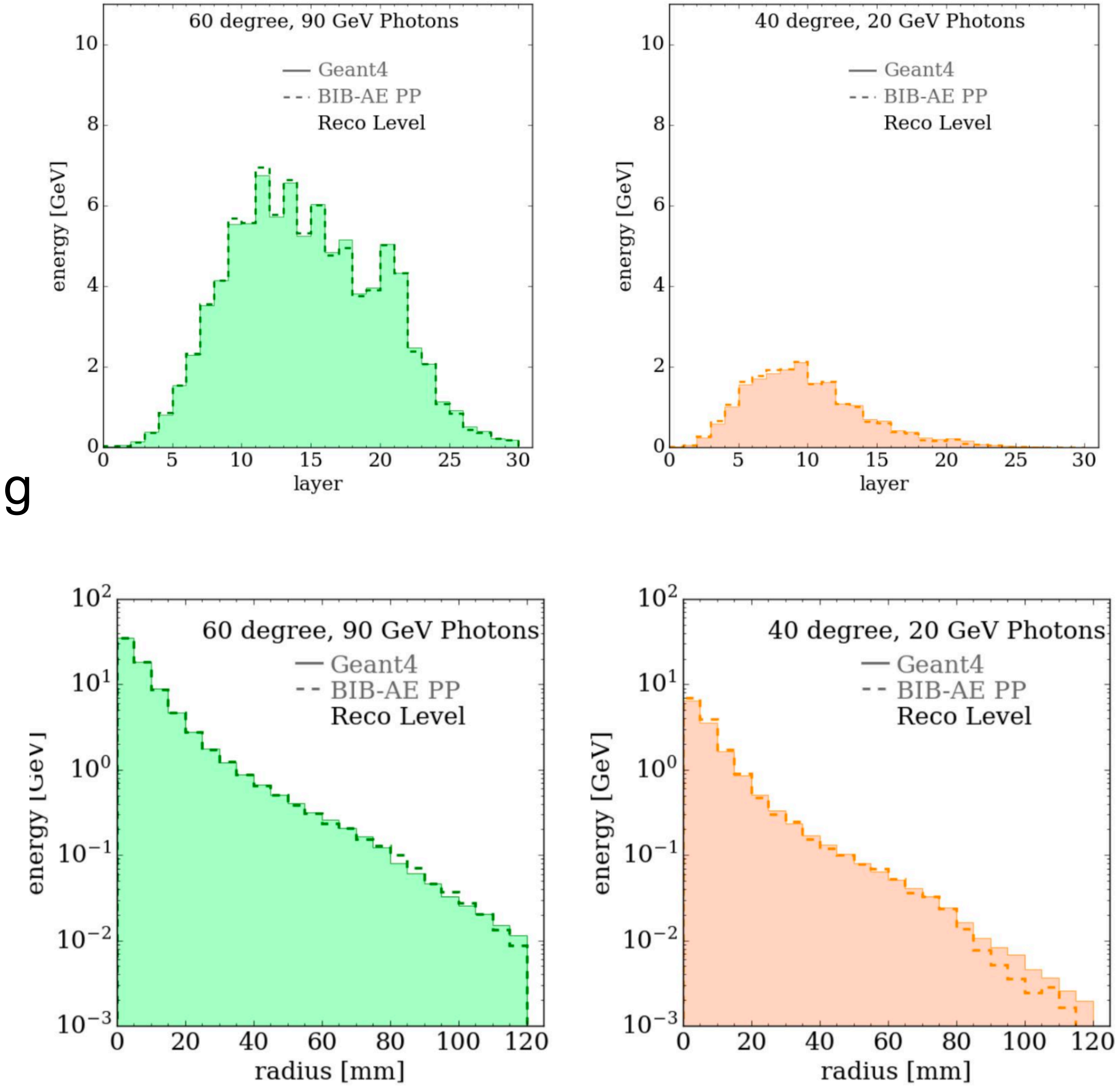
1

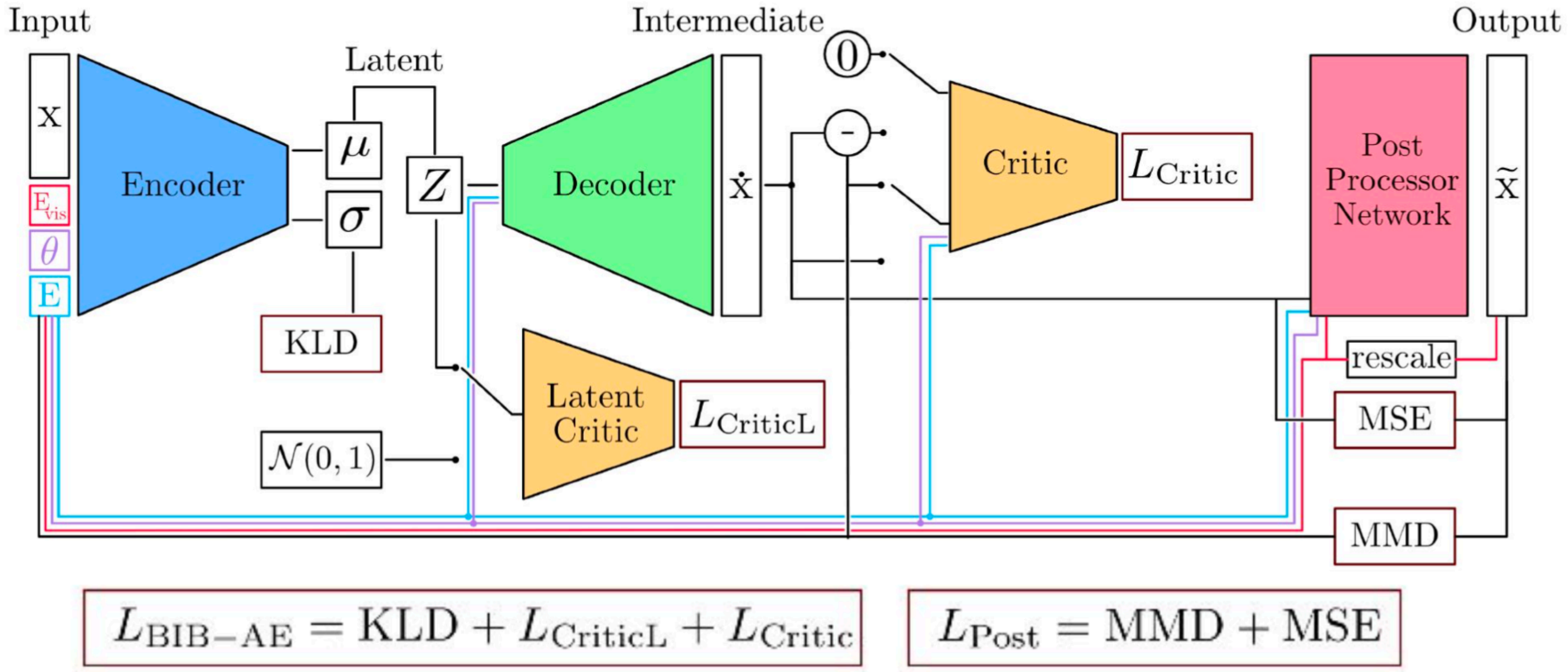
Simulation

Fast Simulation - DESY

BIB-AE With Conditioning

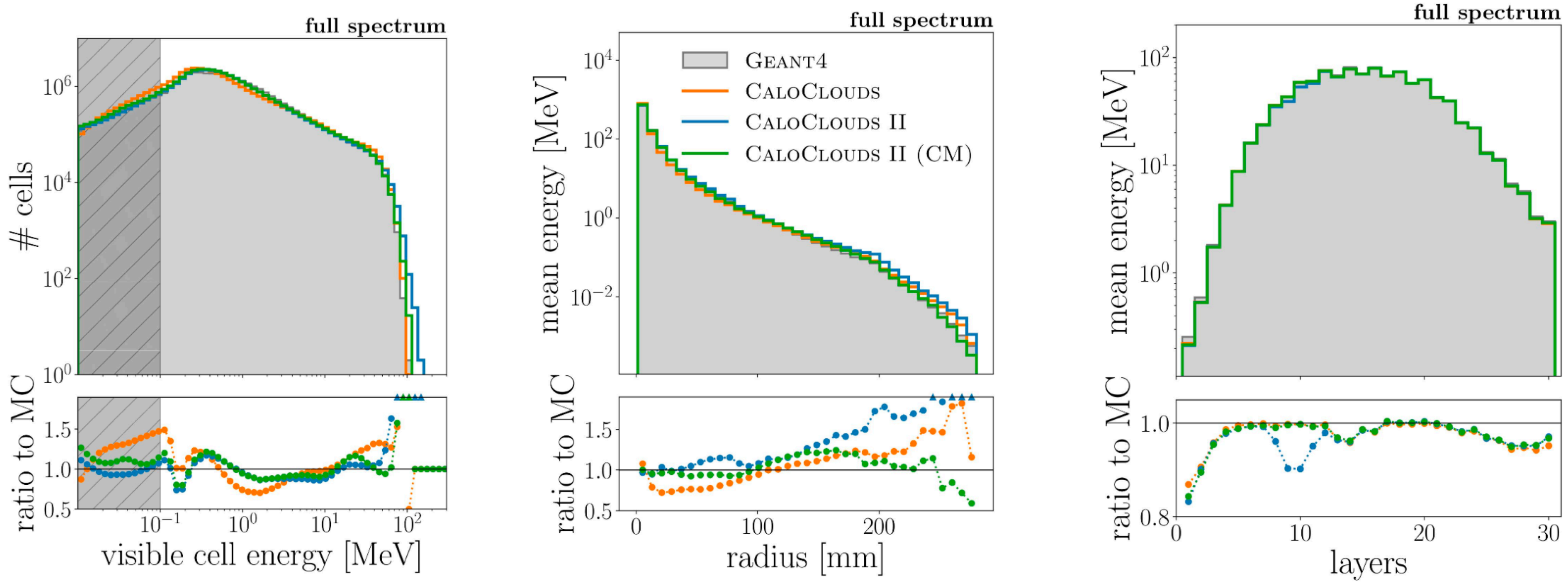
- Condition BIB-AE model on incident energy and polar angle
  - Large training sample - 500k showers
  - Uniform in [10-100 GeV, 30-90 deg]
  - Test/validation samples at dedicated energies and angles
- Now conditioning on 2 angles (θ, φ), which is more challenging

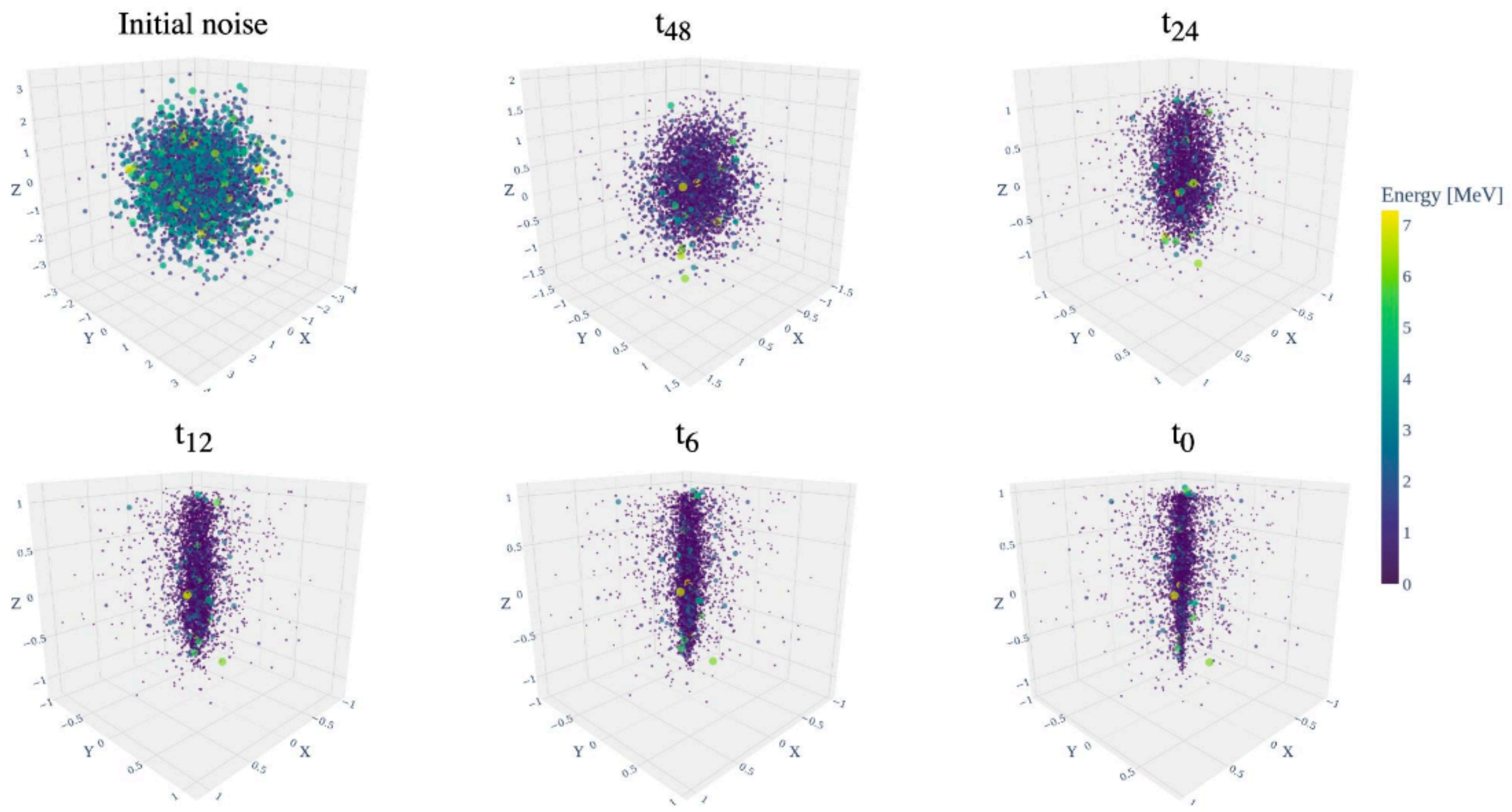




Point Clouds and Diffusion Model

- Point clouds are a good way to handle issues related to details of cell layouts
  - Detach from actual calorimeter geometry
  - They handle sparse data well
  - Model learns to transform noise into realistic shower output

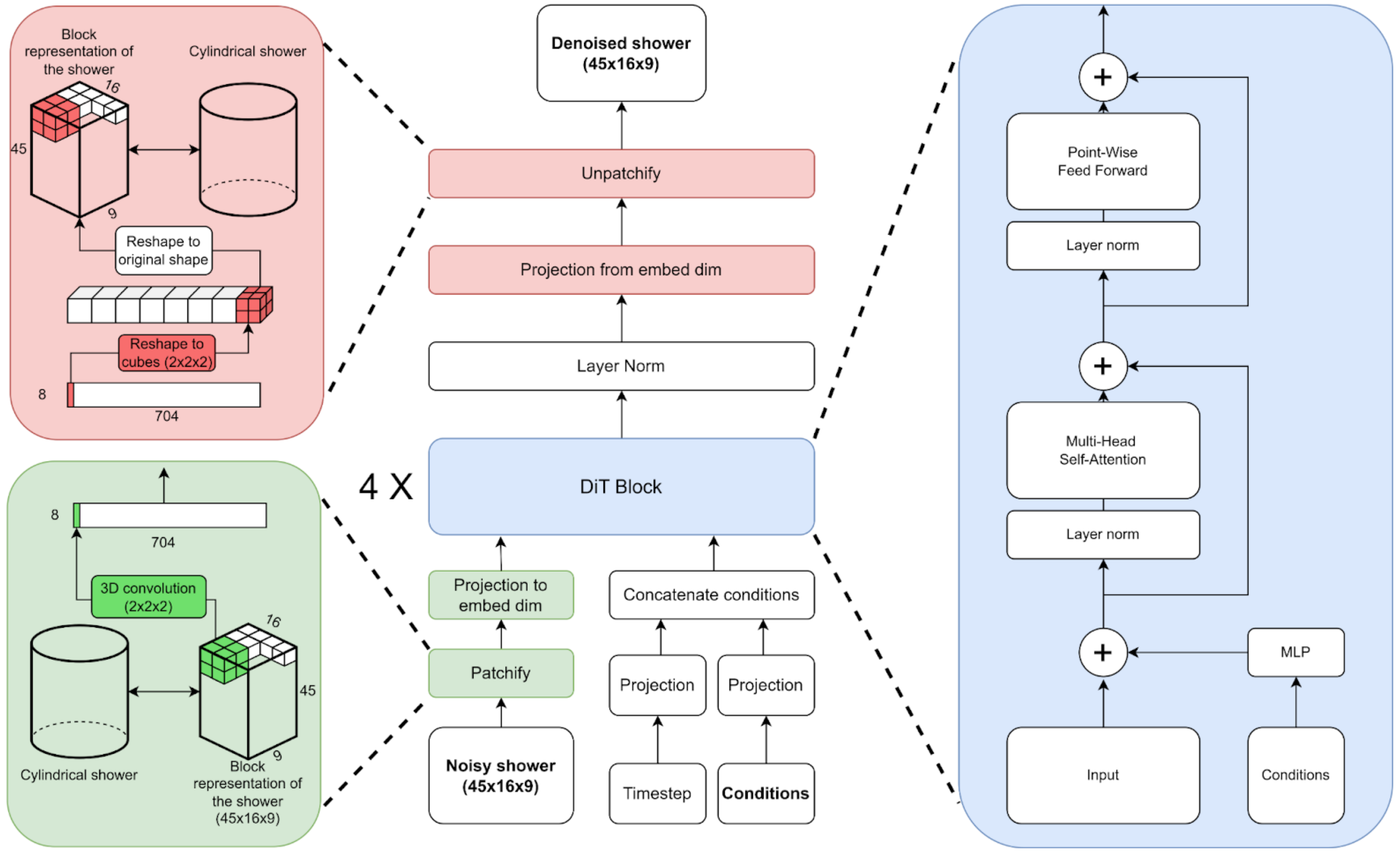


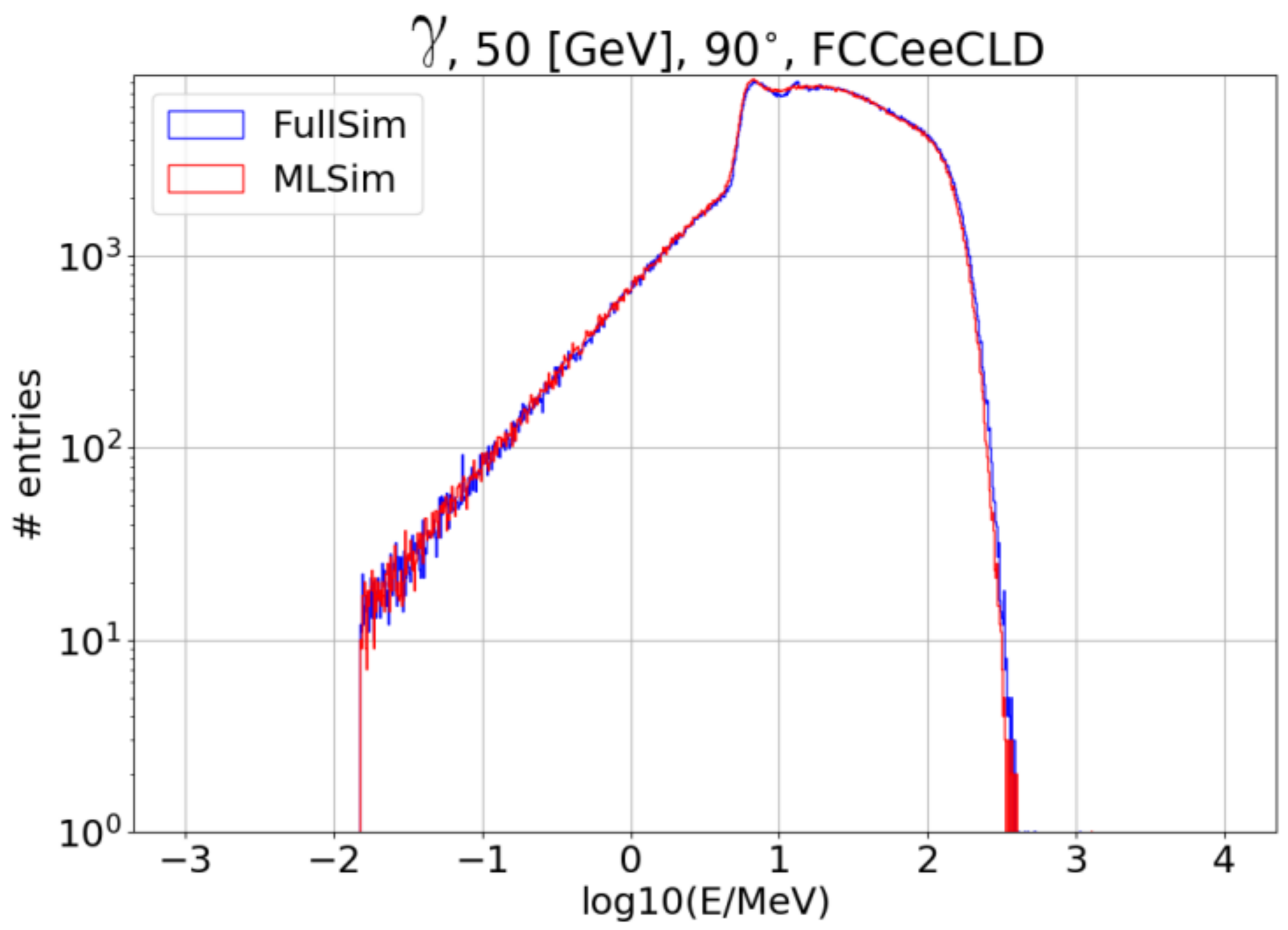


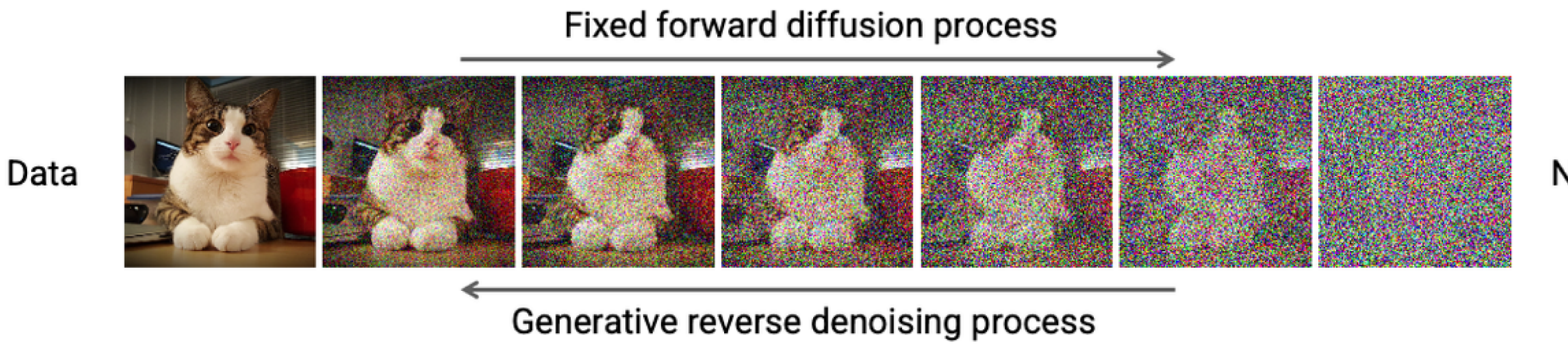
Initial versions of the model were slow (not much faster than Geant4), but speed has now been significantly improved to x46 faster on CPU and x1873 faster on GPU

Fast Simulation - CERN

- CaloDiT
  - Fast simulation model using diffusion in a transformer model
  - Proof of concept integration using Par04 for FCCeeCLD and FCCeeALLEGRO
    - Single γ showers in ECal, 1M samples
    - Energy - 1GeV to 100GeV at a single angle



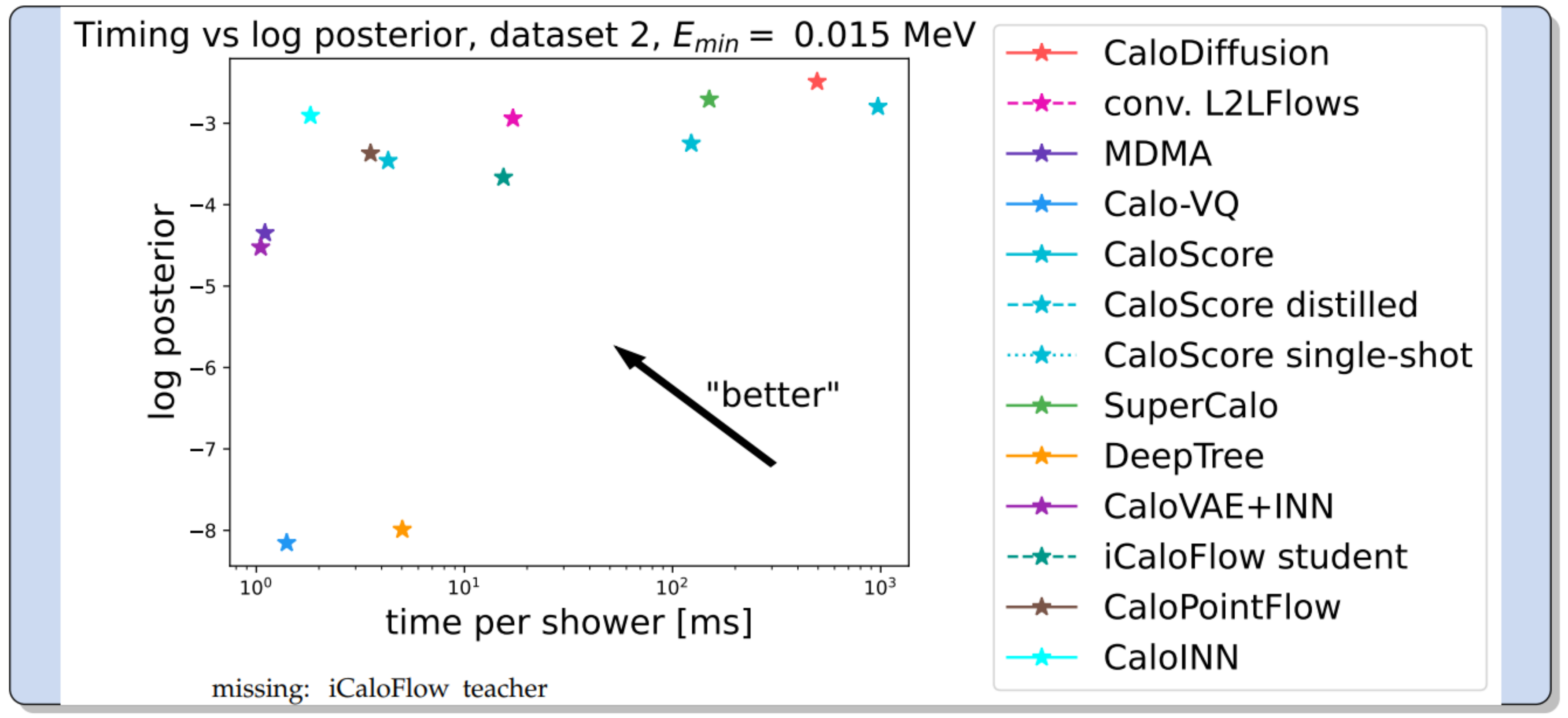



Fixed forward diffusion process
Data
N
Generative reverse denoising process

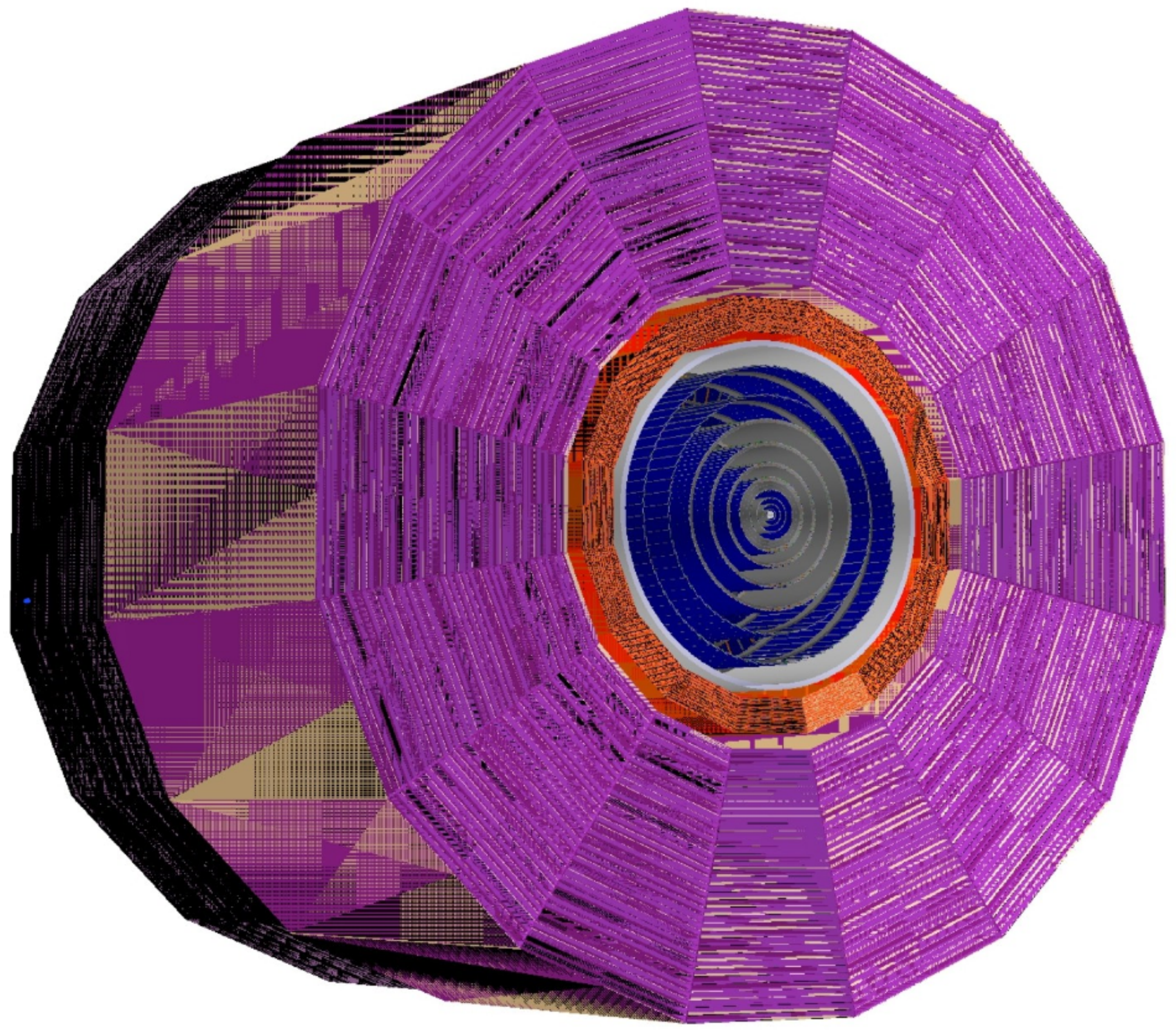
Fast Simulation - CERN

- CaloChallenge
  - ML competition for encouraging development and better understanding of FastSim
  - Fair comparison of models across datasets of varying complexity
  - Workshop held in Frascati, Italy, 30-31 May 2023
  - Results summarised at ML4Jets 2023 and publication is in progress
- Tested overheads of fast simulation in Geant4's Par04
  - Just 0.1ms!
- Open Data Detector
  - Realistic detector geometry for algorithmic research and development purpose
  - Tracker, ECal, HCal are validated
  - Muon system and combined tracking in validation

Generation Times (preliminary!) ds2

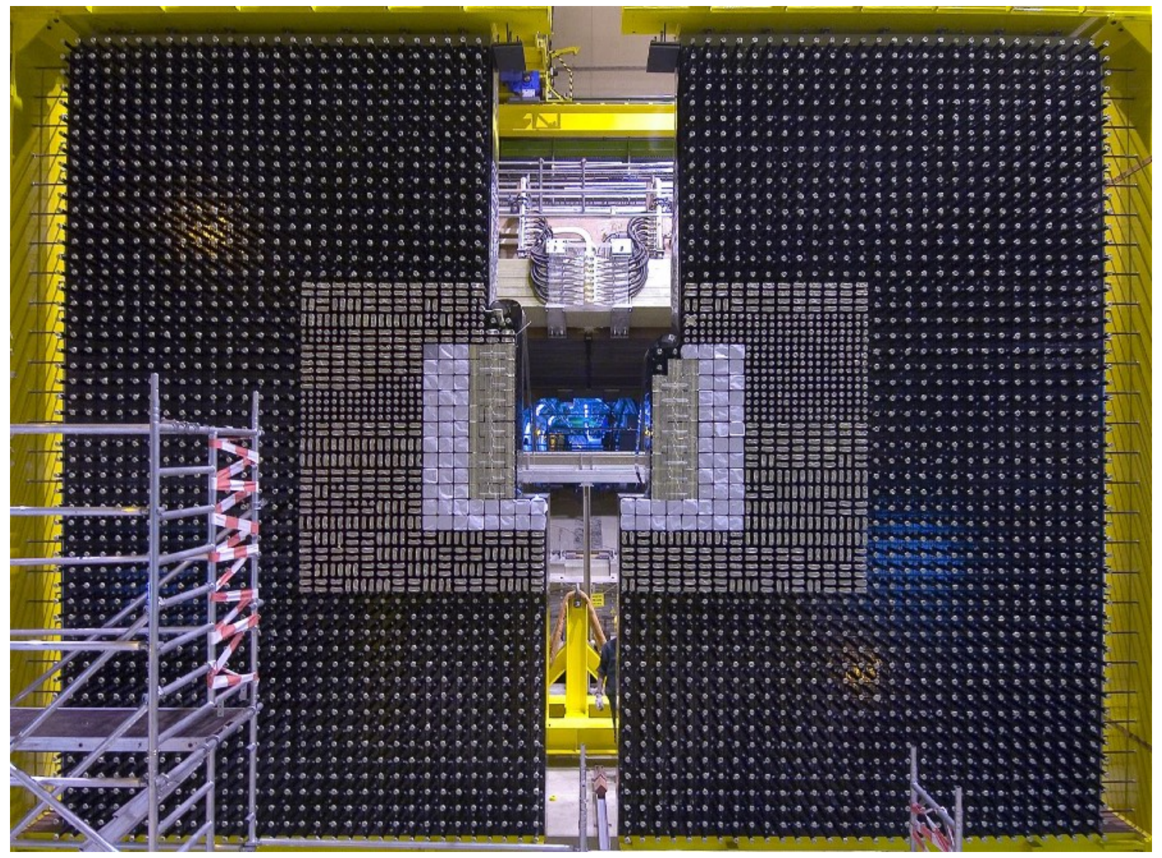


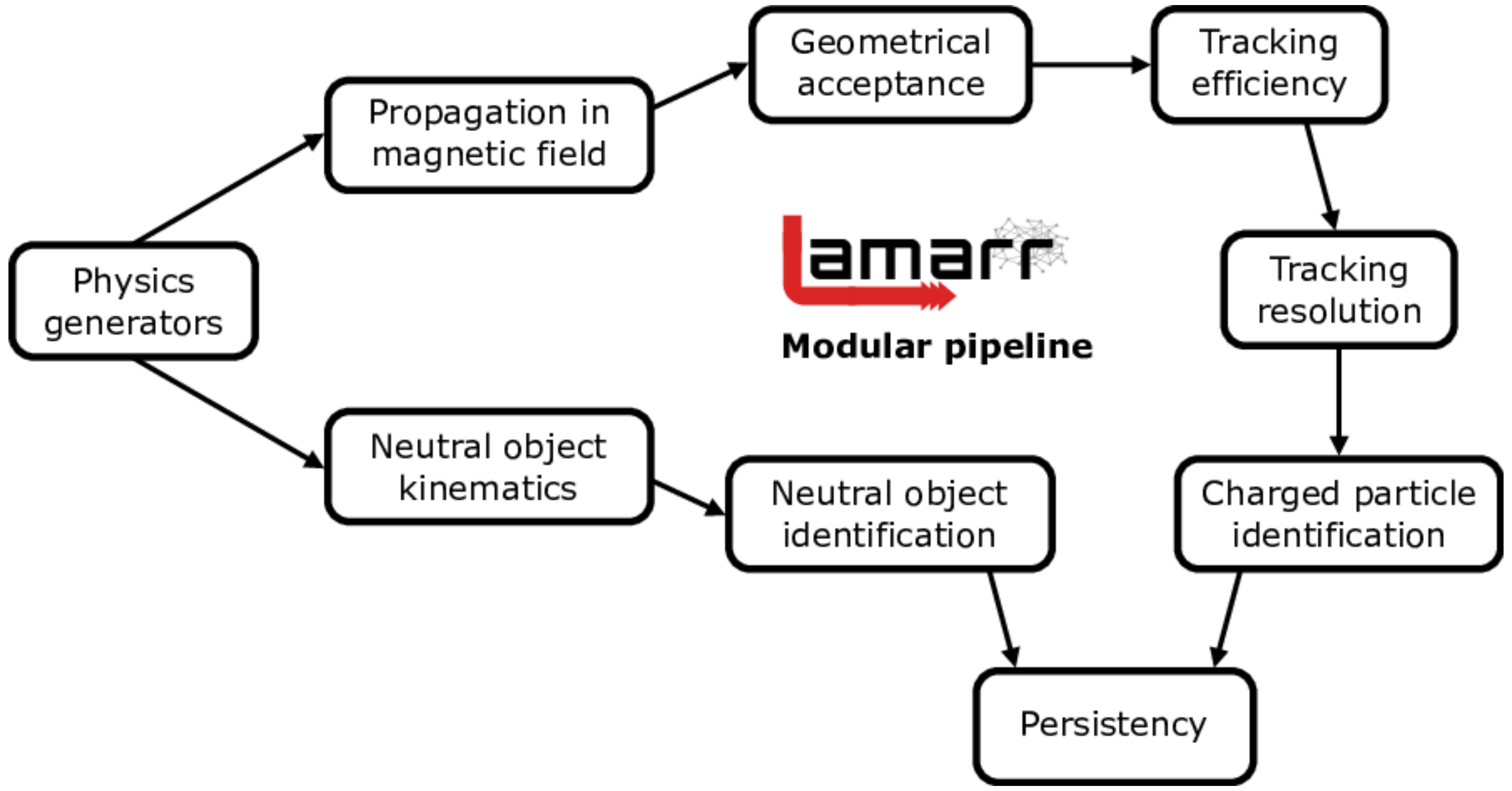
missing: iCaloFlow teacher



Fast Simulation - Manchester

- Work on conversion of LHCb fast simulation package Llamarr, using the Gaussino fast simulation engine
- Focused on LamarrCaloProto (calorimeter simulation in Lamarr)
  - Proof of concept conversion to EDM4hep data model
  - Transition to GaudiFunctional framework and improved thread safety
    - Still need fixes for the random number generator
- Should be on track to wrap up this work in the next year, but personnel initially involved moved on

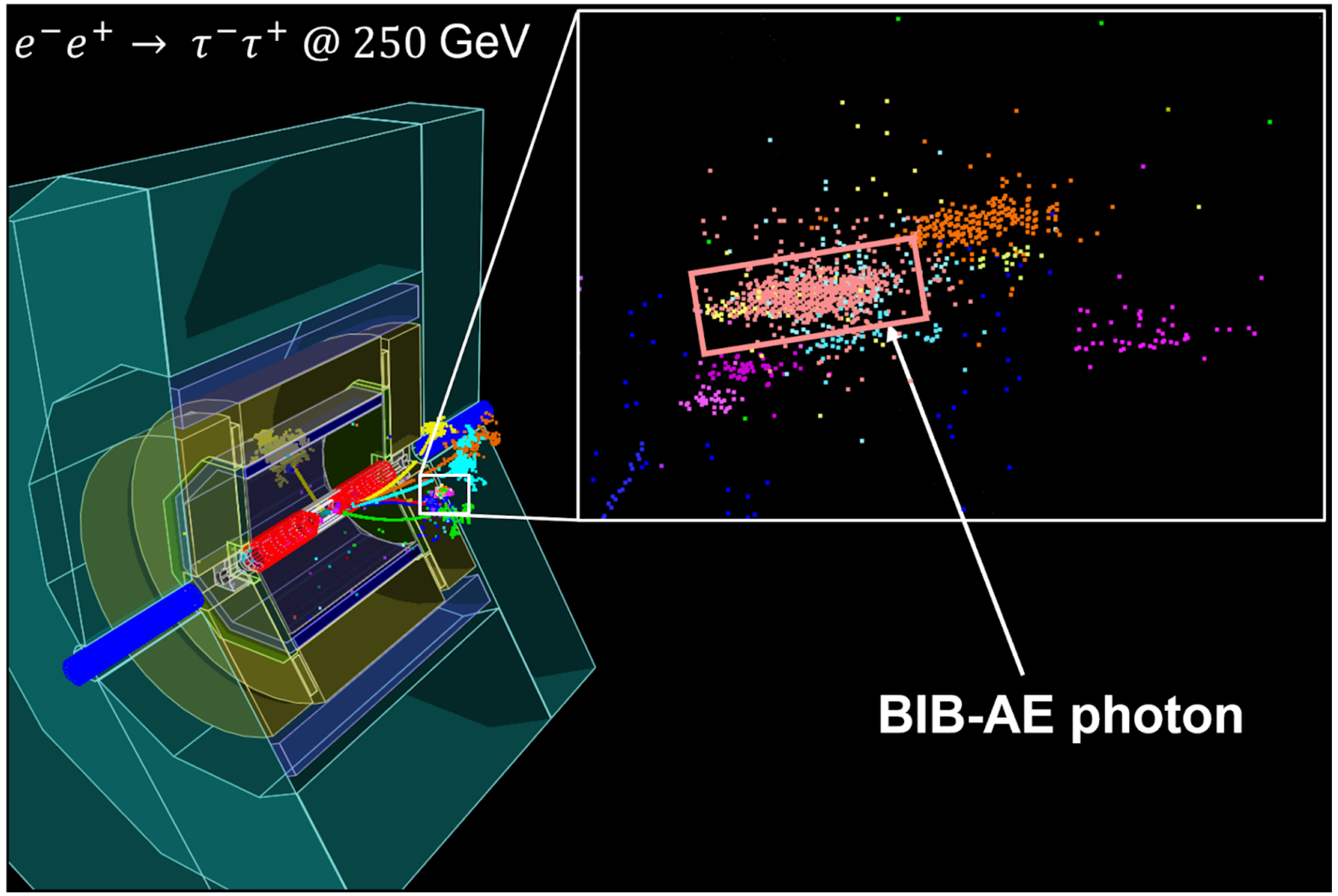



Physics generators
Propagation in magnetic field
Geometrical acceptance
Tracking efficiency
Tracking resolution
Charged particle identification
Neutral object kinematics
Neutral object identification
Persistency
lamarr
Modular pipeline

Faster Simulation

Key4hep Integration

- Link to Key4hep…
  - Fast simulation of photons from the BIB-AE model is *integrated into Key4hep*
  - Using the DDsim package to drive the simulation



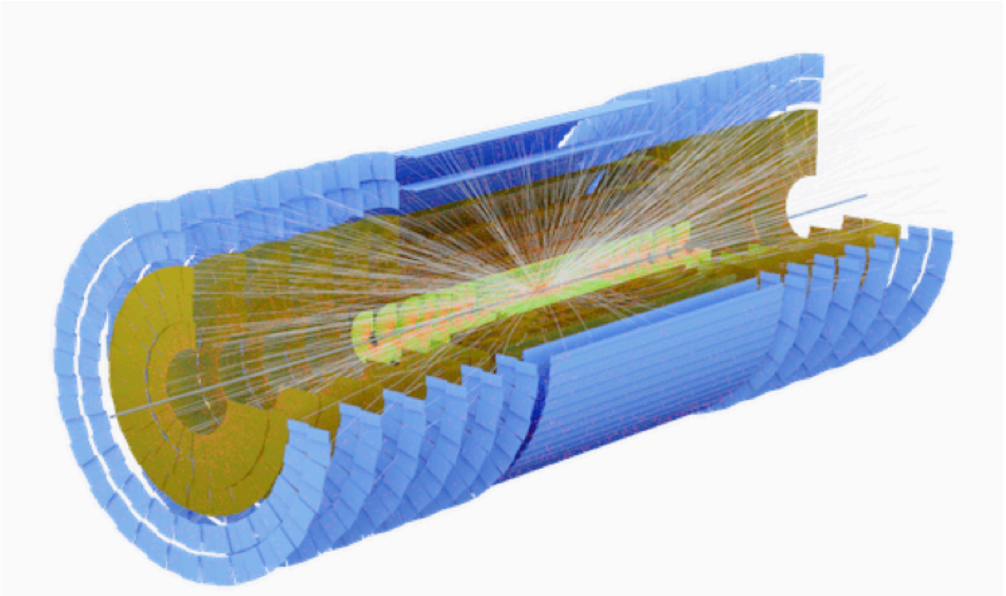
Tracking

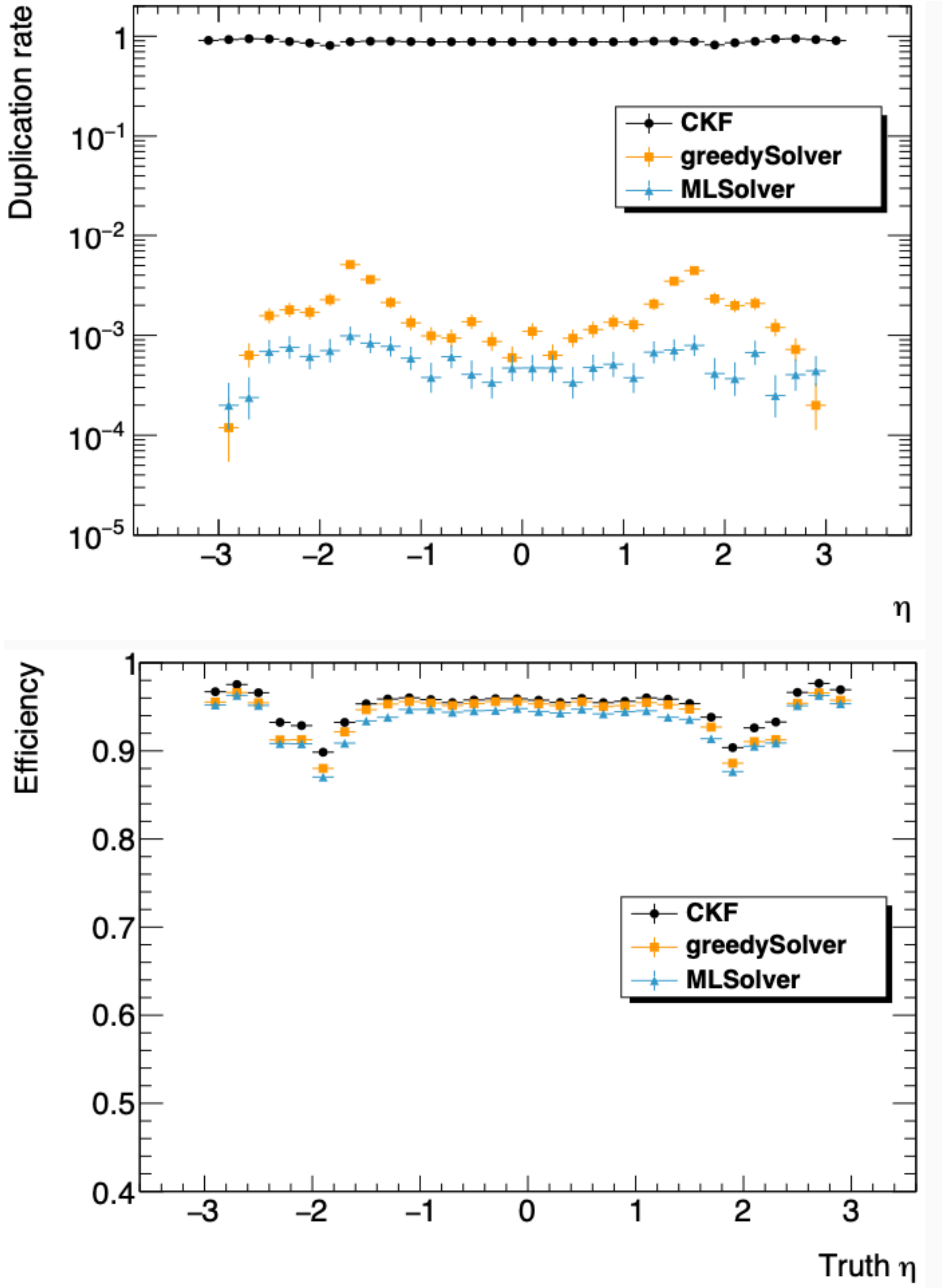
Track Reconstruction

- Develop state of the art tracking for future detectors
  - Working inside the ACTS project that was spawned from ATLAS experiment tracking
  - ACTS now has a wide set of experiments either using or evaluating the toolkit
    - ATLAS, LDMX, ALICE, sPHENIX, FASER, ePIC, CEPC, STCF

Tracking - ACTS Development Highlights

- Switch from 8x8 matrix multiplication to tiled 4x4 technique, allowing linear algebra optimisations
  - Gains +5% in runtime
- Global χ^2 fitter and Gaussian Sum Filter implemented
  - Important for best possible track fits for, e.g., electrons
- Public track EDM + PODIO/EDM4hep support
  - Links to EMD4hep changes allowing better description of TrackerHits
- Geometry support for GDML
- Improvements in Open Data Detector (work in conjunction with simulation team)

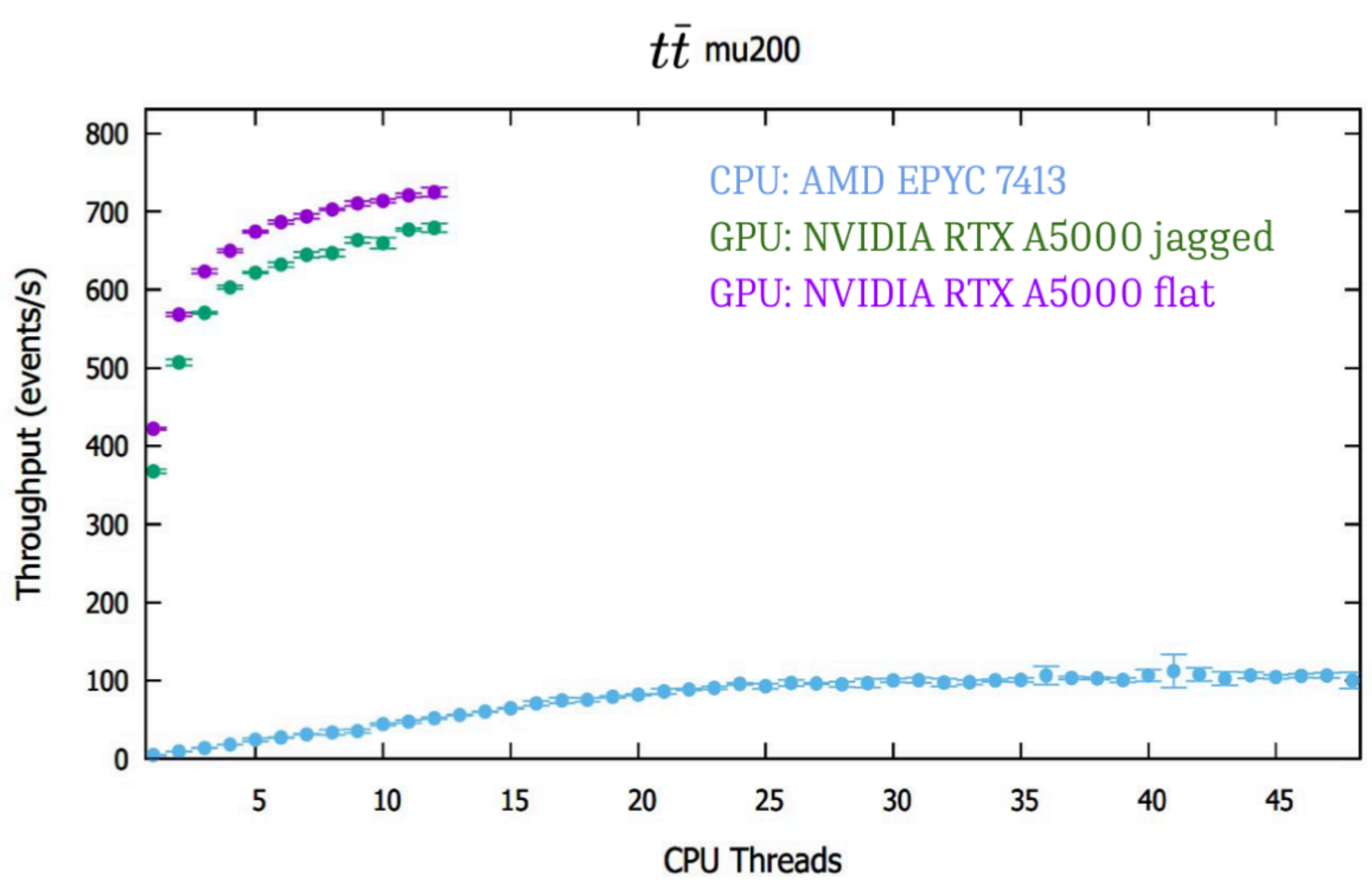


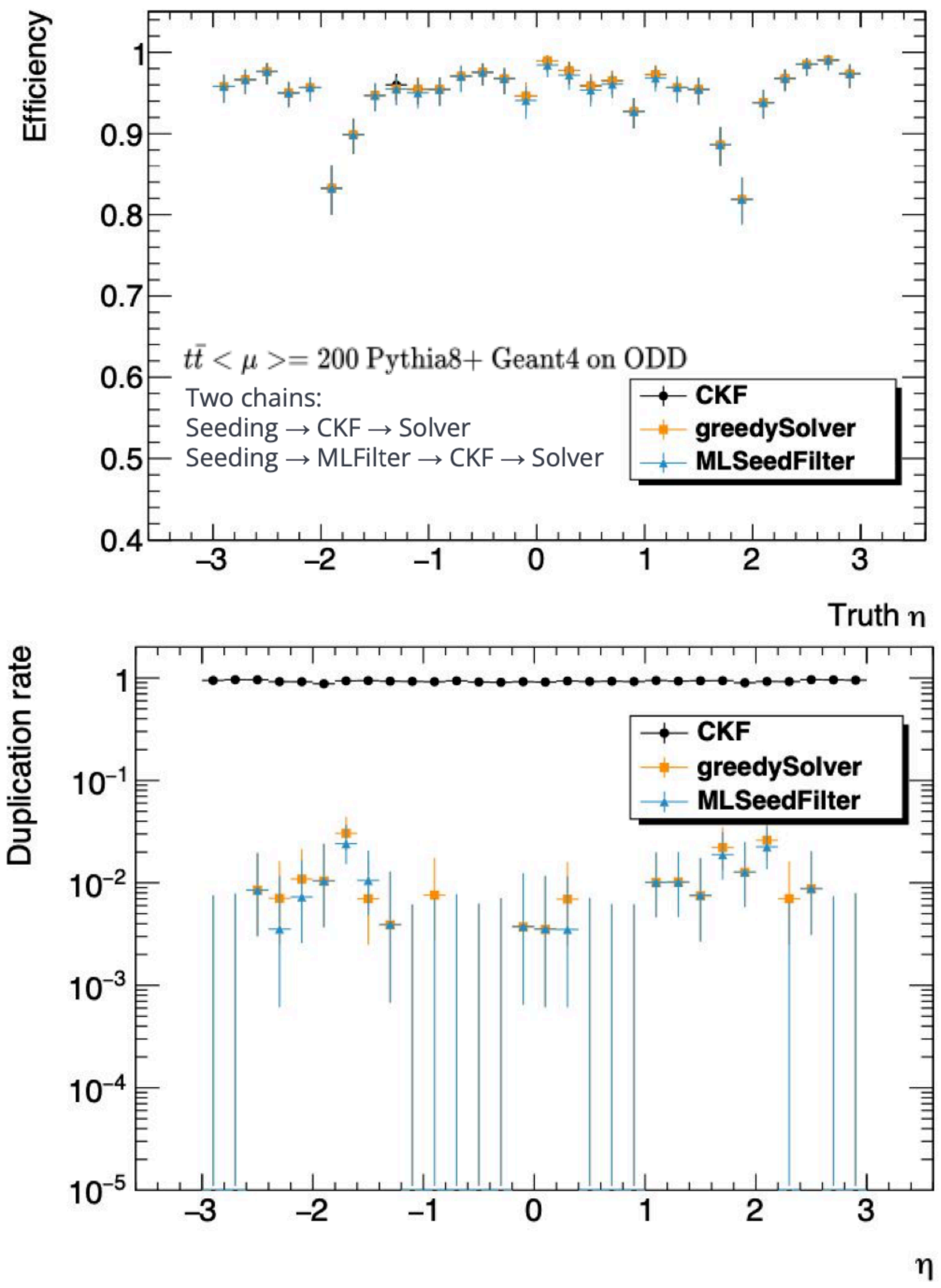


- Machine learning ambiguity resolution

ACTS R&D Lines

- Track seeding
  - ML seed filtering prototype speeds up track fitting by ~50%
    - Reduces tracks per event by ~2.6, but with only a tiny efficiency loss



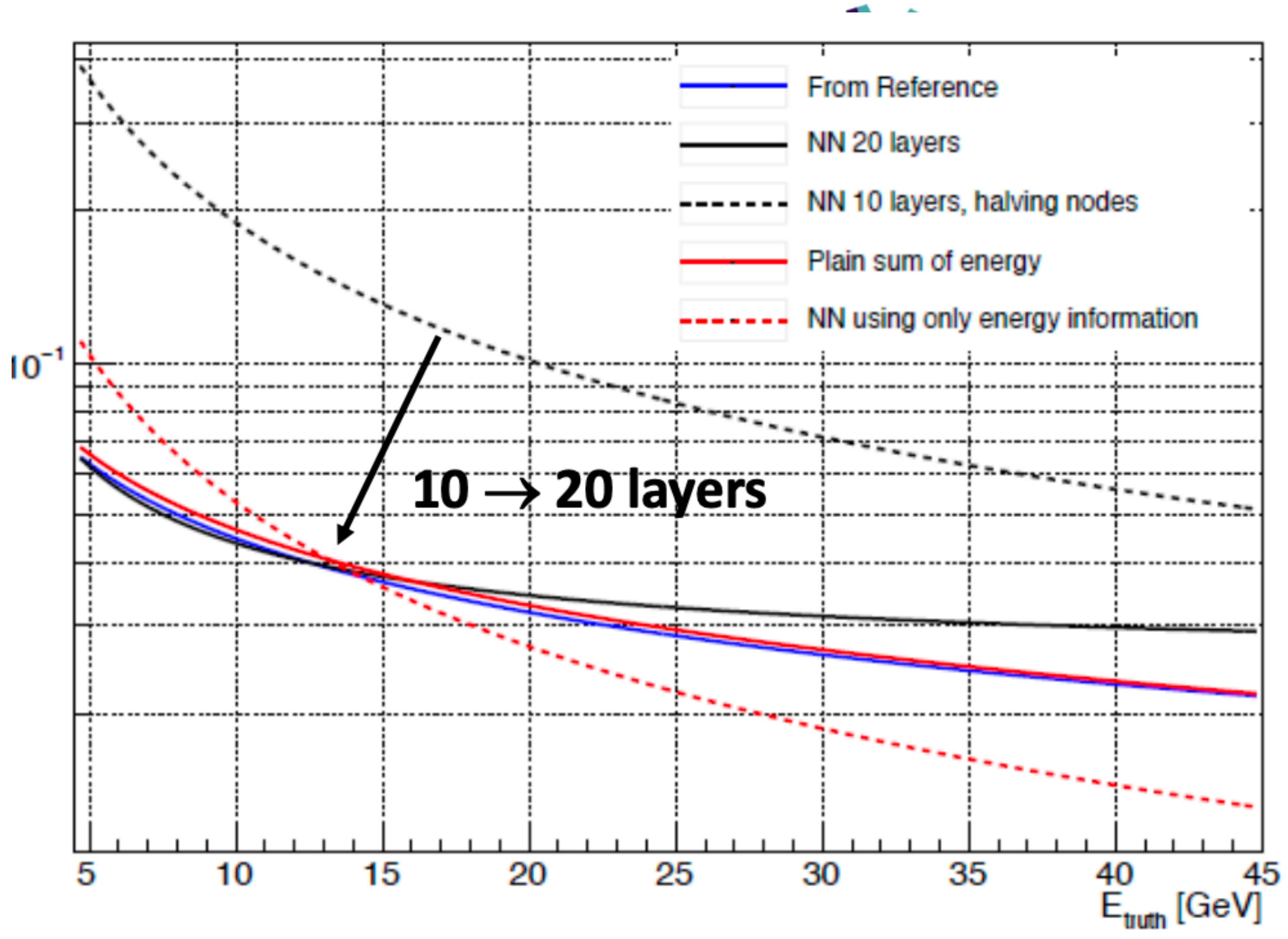


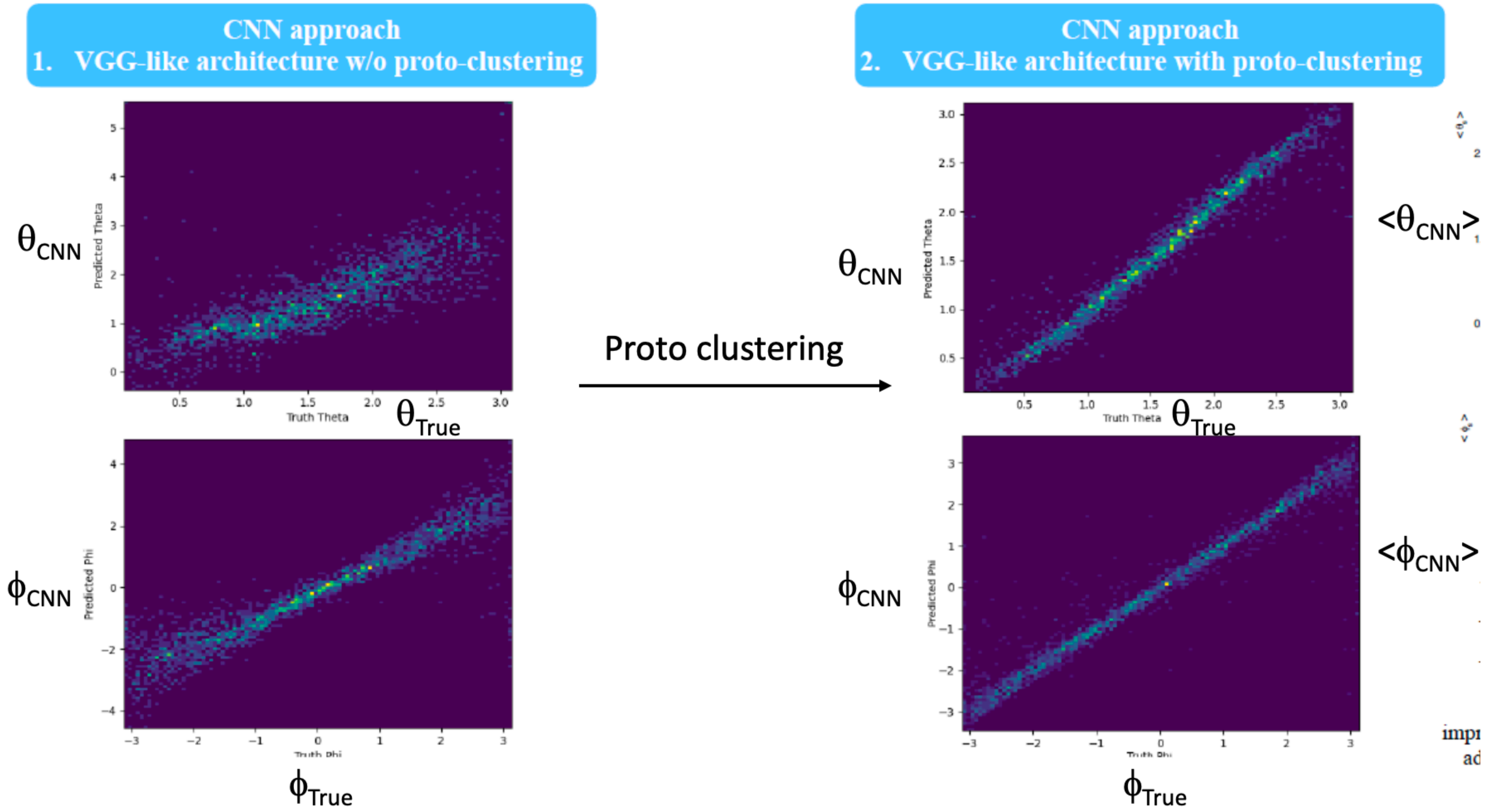
- GPU based track seeding offers substantial speed-ups for high pileup events

Particle Flow

Dual Readout Calorimeters

- Started investigation into machine learning based reconstruction
  - Idea was to take energy deposits and train a neural network that can maximise the energy resolution
- However, results have been disappointing!
  - Various deep neural network (DNN) models were tried for learning to predict electron energy
    - The problem seemed too complicated for the model to learn: bending in B field, radiation emission, fibre geometry
  - Tried a convolutional neural network (CNN) to predict the angular resolution
    - Results were very poor - “improved” by proton-clustering, but CNN adds little
- Now re-scoping the project to try to use traditional reconstruction and then see if a NN can add something extra




CNN approach
1. VGG-like architecture w/o proto-clustering

CNN approach
2. VGG-like architecture with proto-clustering

APRIL PFA for Hadronic Jets

- SDHCAL needed corrections for both θ and φ
  - Without these E_{rec} was too low
    - Now this is corrected
  - New git repository for SDHCAL content
- Added an SDHCAL version of DDMarlinPandora
  - Can be compiled in Pandora mode or APRIL mode
    - SDHCALContent compatible with Pandora LCContent and APRILContent
- Next steps
  - SDHCAL K-long simulation at higher energy, calibration of SD energy reconstruction
  - Technical improvements to reuse Pandora plugins with APRIL; improved runtime integration for DDMarlinPandora

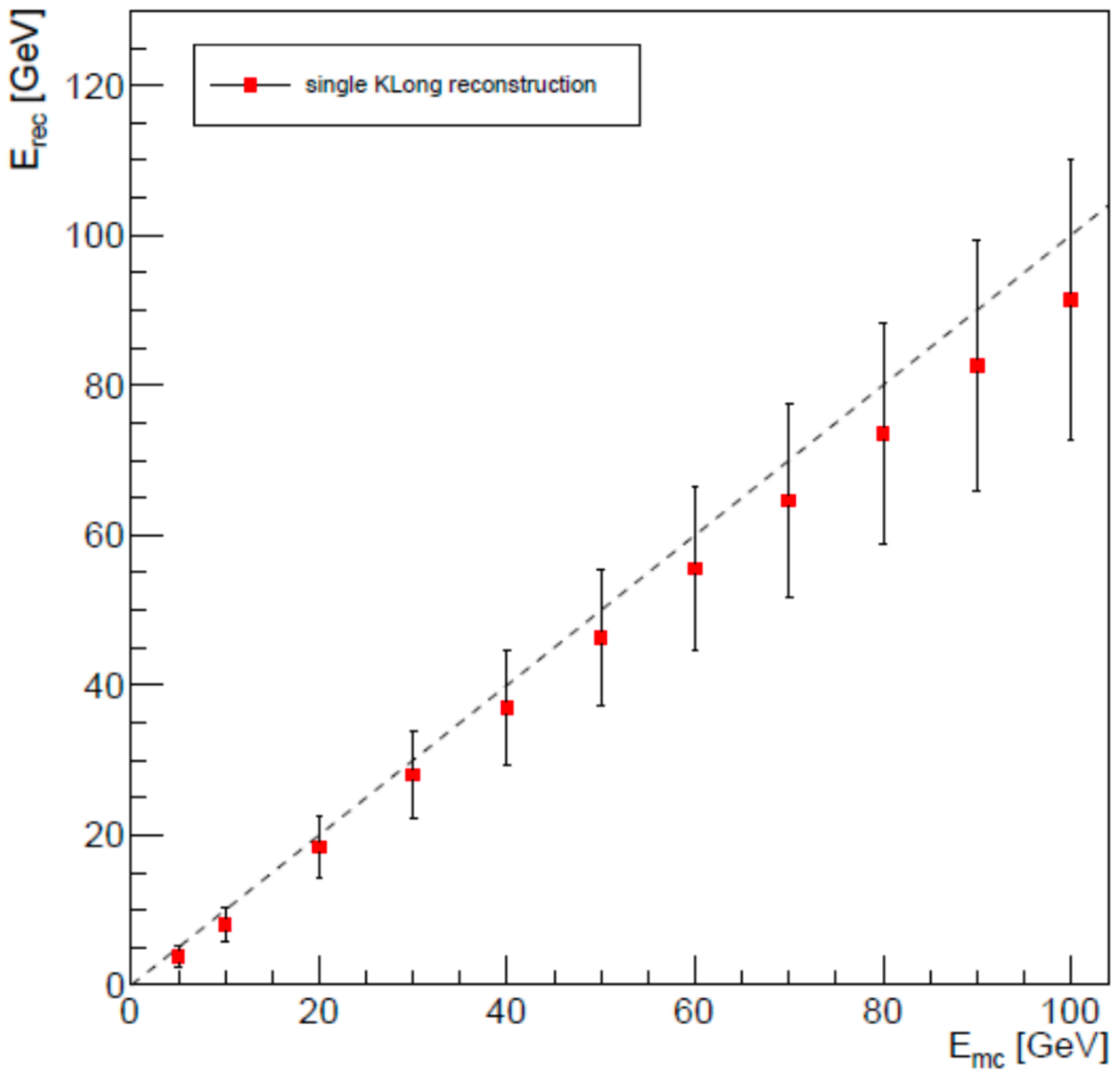


Figure: E_{rec} before correction

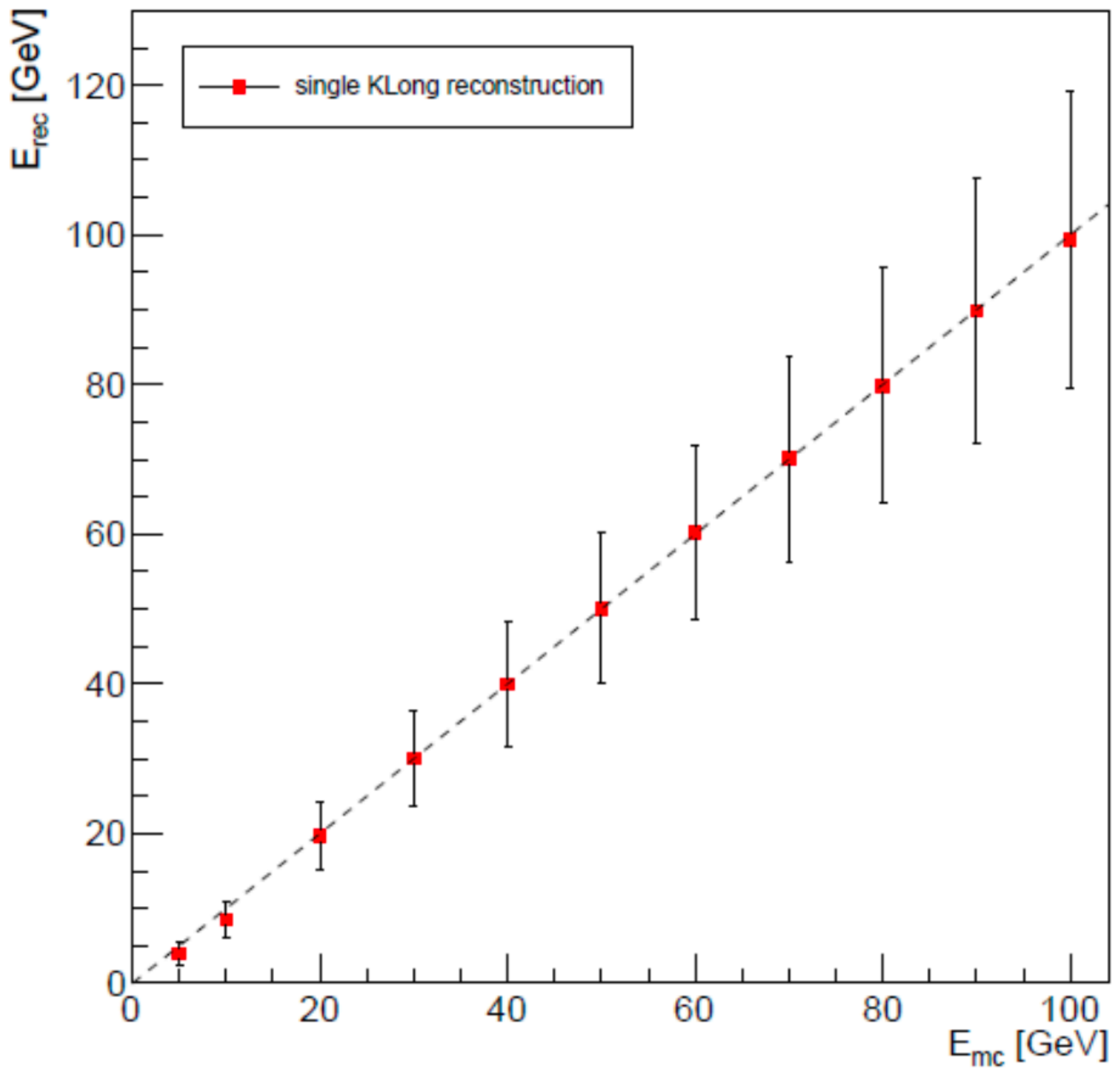
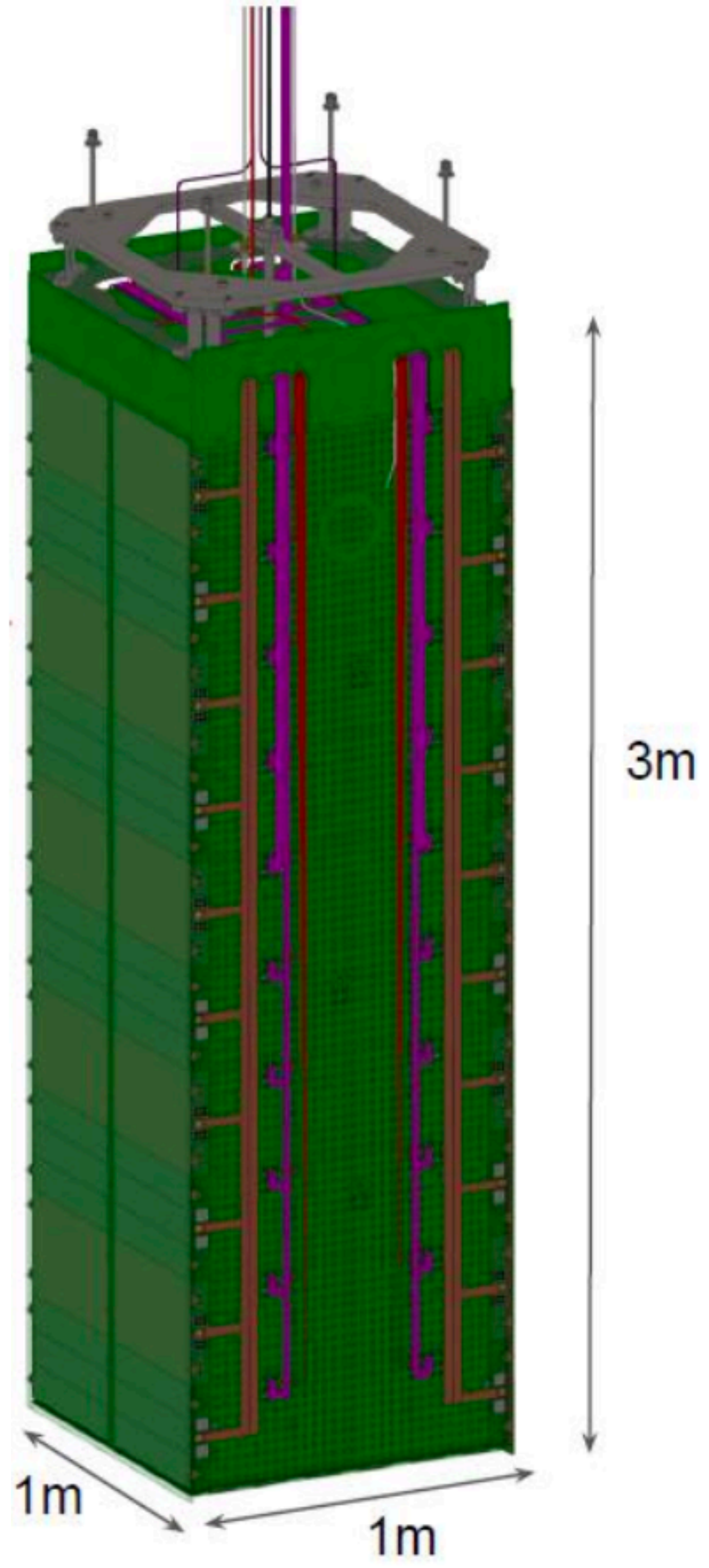
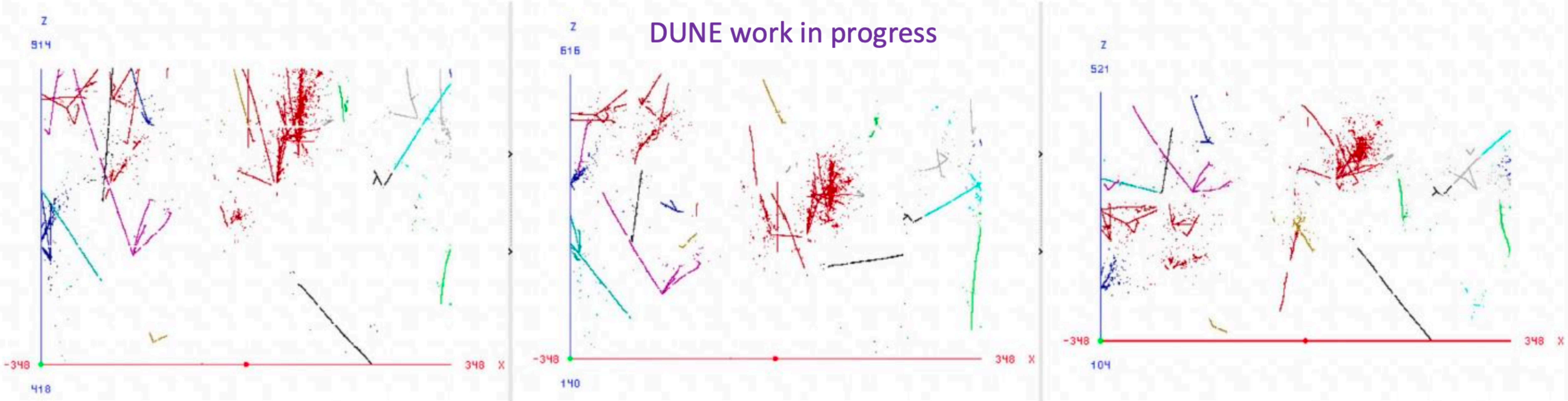


Figure: E_{rec} after correction

DUNE Near Detector Reconstruction

- DUNE ND is 7x5 array of 1x1x3m LAr modules with 3D pixel readout
- Expectation of 50ν interactions per second
  - Can split complex spills into slices with ~1ν per slice
  - Search for the main vertex to improve particle flow



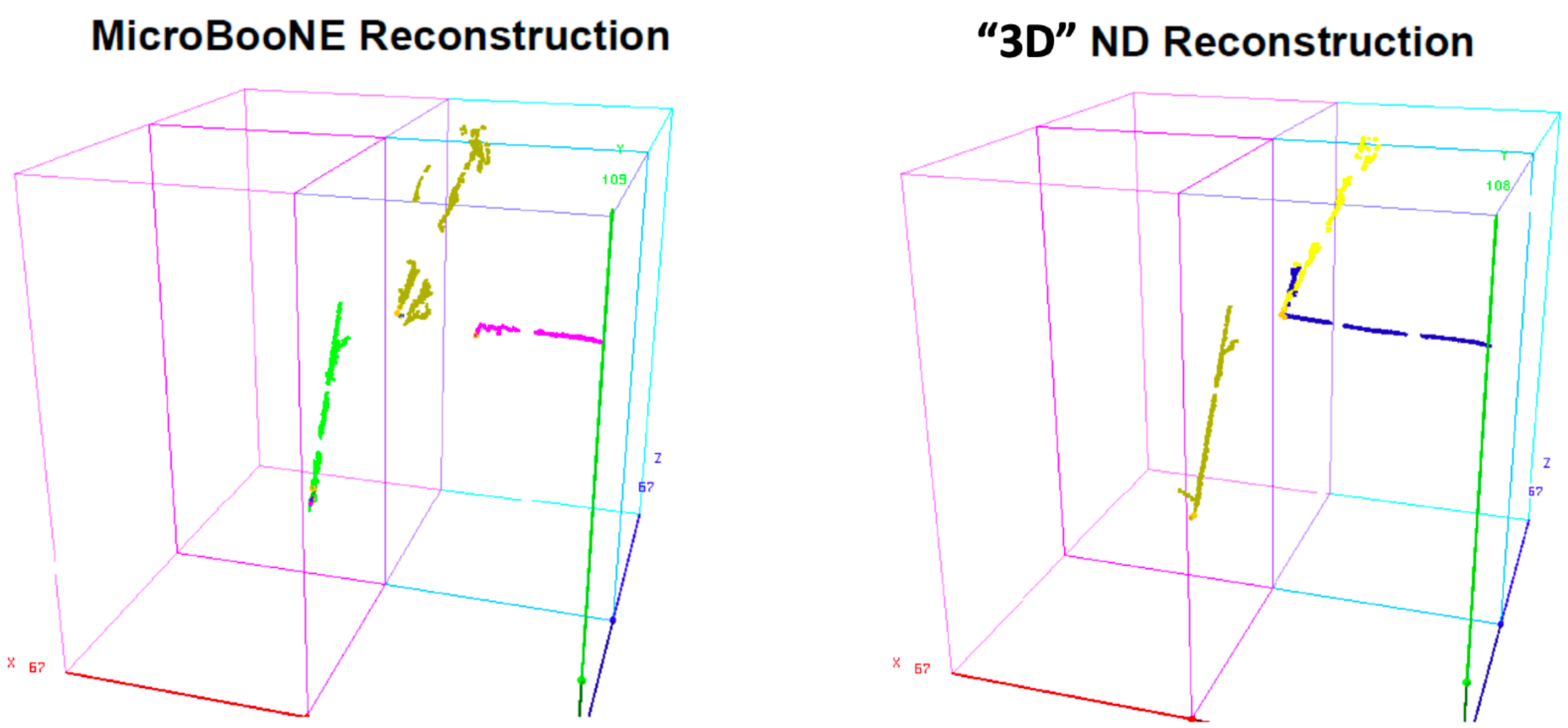


DUNE work in progress

2D projections of reconstructed PFOs, **1 colour = 1 slice**

DUNE ND in 3D

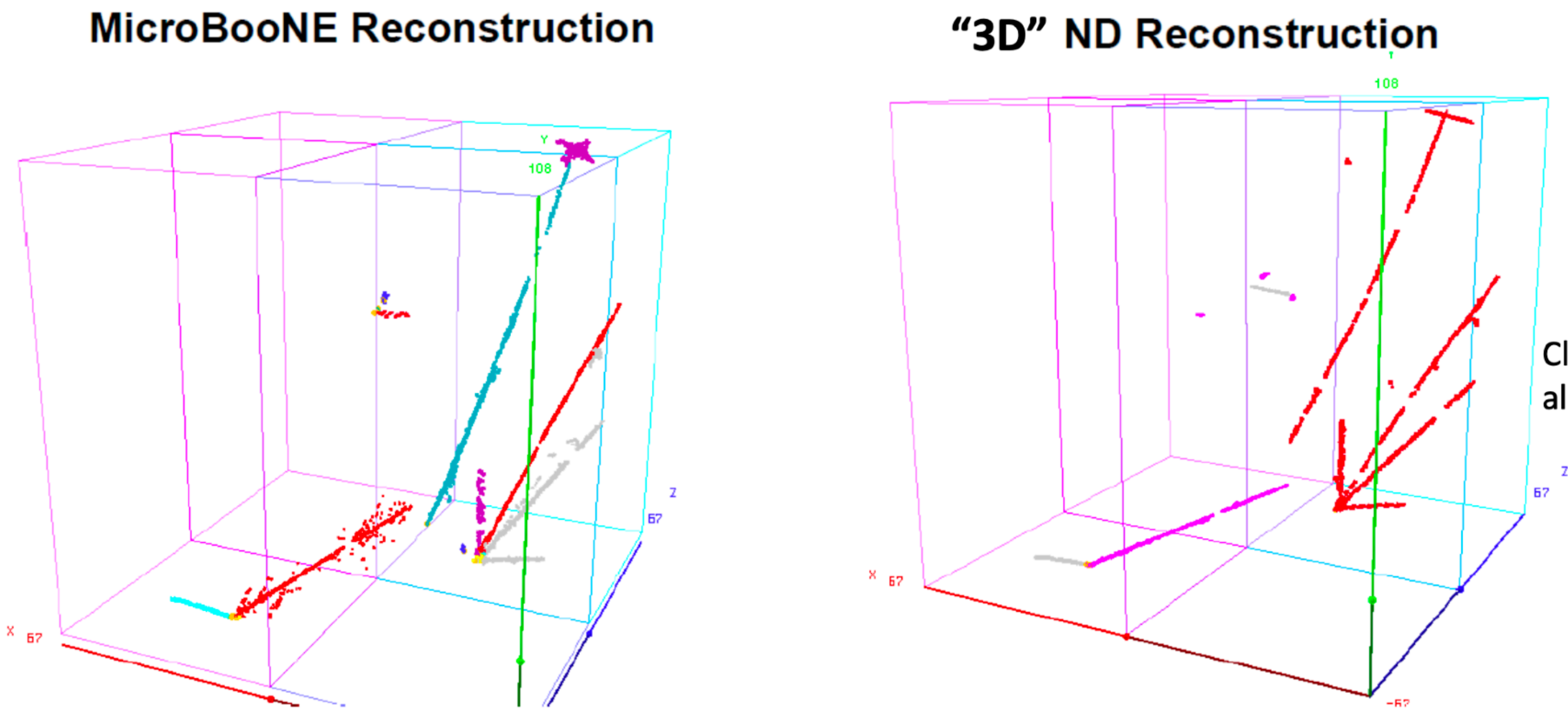
- Cluster initial hits in 3 dimensions
- Merge and refine clusters using current 2D algorithms (y coordinate ignored - to fix!)
- Create particle flow objects and match back into 3D



MicroBooNE Reconstruction

“3D” ND Reconstruction

DUNE work in progress



MicroBooNE Reconstruction

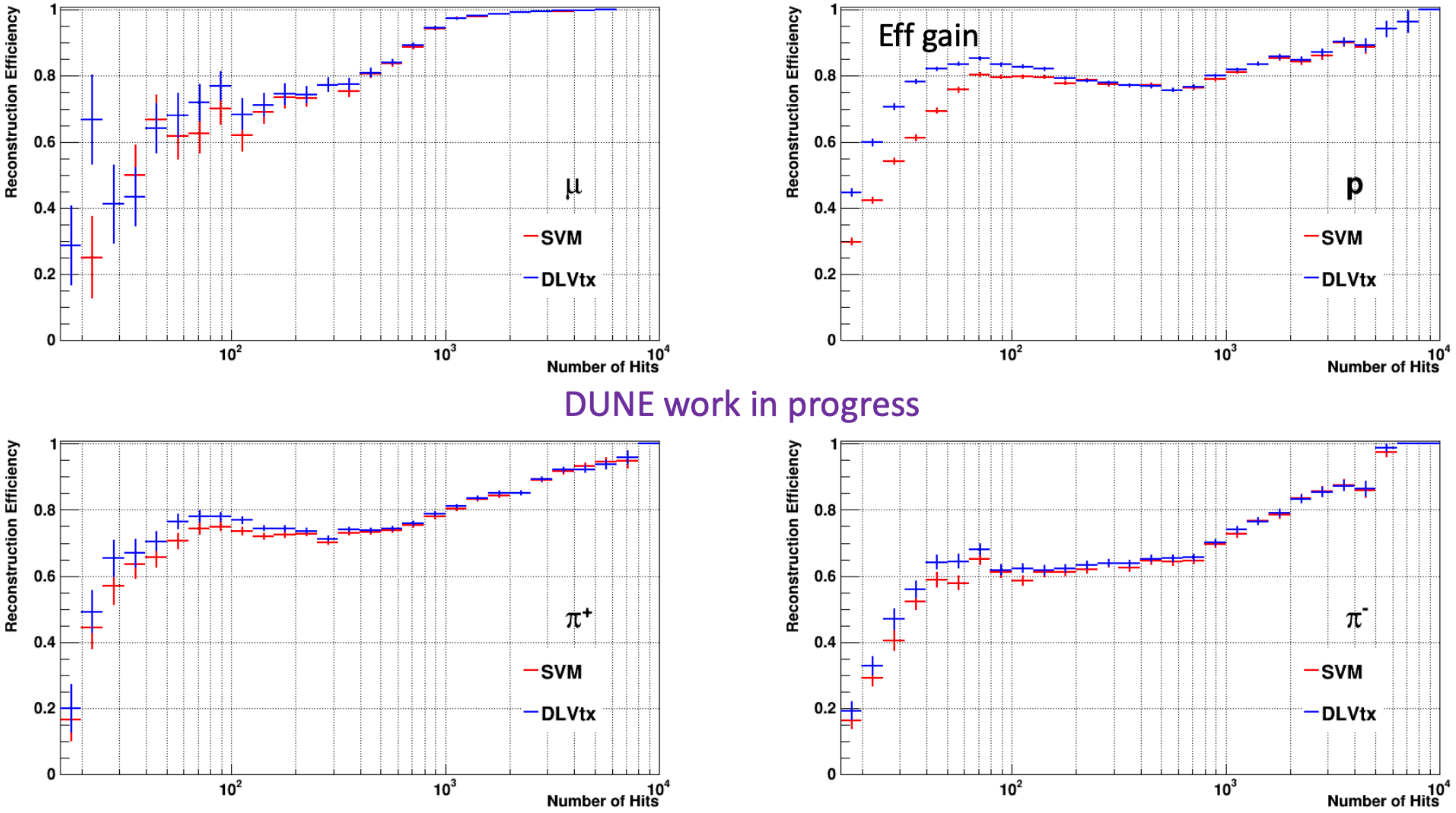
“3D” ND Reconstruction

Clusters overlap along y projection

DUNE work in progress

Deep Learning for Vertexing

- Train a neural network on 50k ν_e images in U, V, W 2D projections
- Good results for vertexing translates into better hit reconstruction efficiencies



DUNE work in progress

SVM: MicroBooNE support vector machine, DLVtx: pytorch ND deep learning vertexing

Hackathon and Conclusions

Software Hackathon

- We took advantage of being together to have a hackathon, focusing on simulation and Key4hep
- We worked on…
  - Caloclouds model export to pytorch
  - Using CEDViewer for the ODD
  - OS X port of Key4hep
  - DDFastShowerML added to Key4hep
  - Pipeline to publish PODIO documentation
  - Write a Gaudi algorithm for k4PandoraPFA
  - Adding CaloDiT model into Par04 example

Conclusions

- WP12 is progressing well overall
  - Significant progress in the last year in almost all tasks
- We should be on-track to complete all of our deliverables on time
  - We remain attentive to ensuring that everything is on track in the home straight