AIDAinnova - WP 12
Software for Future Detectors

Annual Meeting 2023

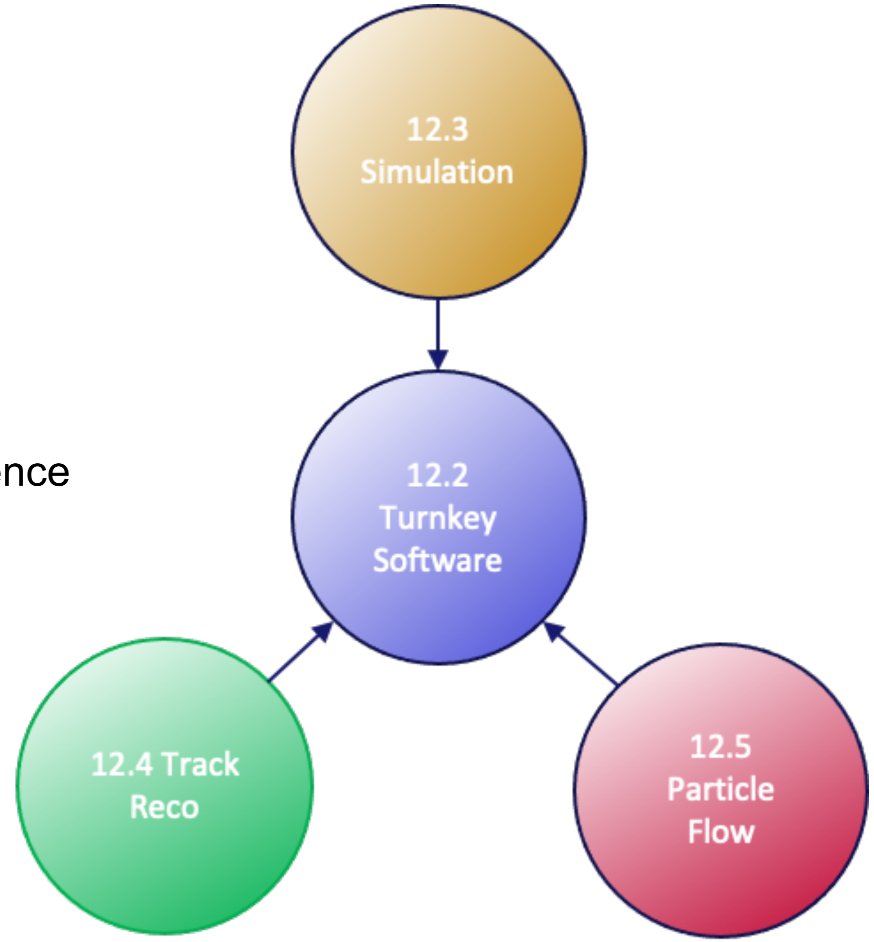
Valencia

F. Gaede, DESY, G. Stewart, CERN
26.04.2023

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

WP12 Structure

- **Task 12.2. Turnkey Software**
  - Turnkey Software Stack, for physics and performance studies, EDM4hep, PODIO and Digitisation toolkit
  - R&D study on frameworks to manage heterogeneous resources
- **Task 12.3. Simulation**
  - Fast simulation techniques integrated into Giant
  - Machine learning based calorimeter simulation toolkit for training and inference
- **Task 12.4. Track Reconstruction**
  - complete track reconstruction with ACTS composable algorithms and for heterogeneous computing
  - Machine learning reconstruction algorithm for MPGD detectors
- **Task 12.5. Particle Flow Reconstruction**
  - PFA algorithms for DUNE and dual-readout calorimeters, APRIL PFA for hadronic jets



Partners and Task Leaders in WP12

- Task 12.1. Coordination and Communication **(CERN, DESY)**
  - G.A.Stewart, F.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
  - T.Madlener, A.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
  - A.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
  - H.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
  - J. Back, J. Marshal

Deliverables and Milestones

in WP12

Deliverab le	Title	Due Date
D12.1	Turnkey Software Stack (Key4hep)	46
D12.2	Fast shower simulation in Geant4	45
D12.3	ACTS tracking algorithms	43
D12.4	PFA reconstruction	45

- all four milestones have been met on time end of last year/ beginning of this year
- on a good track towards final deliverables at the end of the project …

Milest one	Title		Due Date
MS48	LC reconstruction prototype in Key4hep	Reproduce similar detector performance as achieved with the current framework	21
MS49	Prototype of ML based shower simulation	Runnable example code that simulates part of the showers with ML algorithms	22
MS50	ACTS tracking algorithm prototypes	Runnable test cases which demonstrate algorithm functionality on benchmark data from TrackML	23
MS51	New PFA prototypes	Runnable test cases which demonstrate algorithm functionality on benchmark data	23

Programme in Valencia

- detailed reports in WP12 session on Monday
    - excellent progress in all tasks

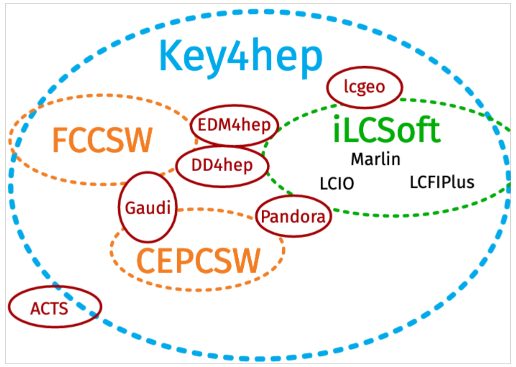
- also used opportunity to have a **hackathon** here in Valencia addressing pressing issues in person

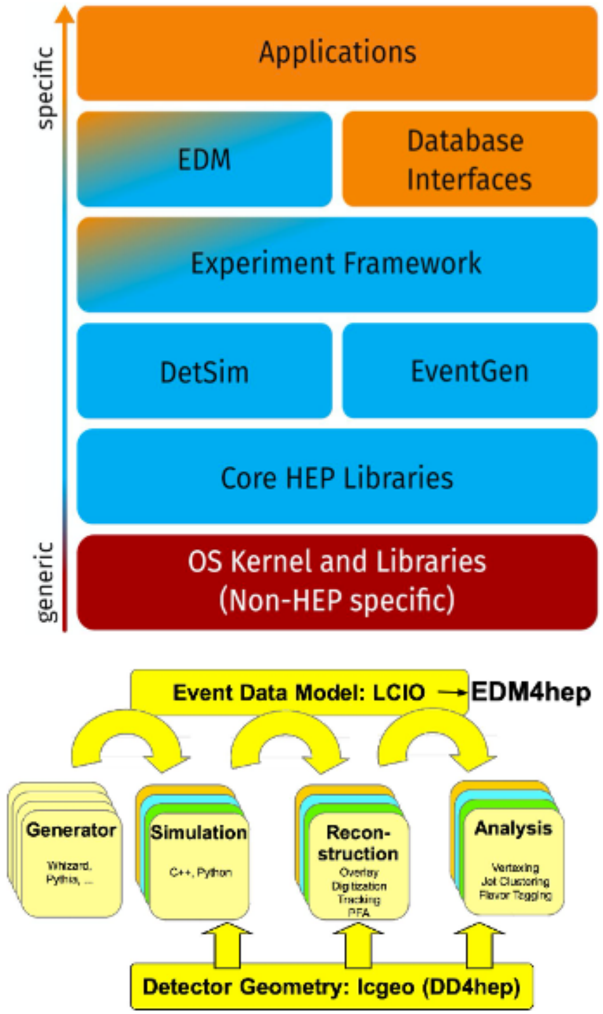
Introduction	*https://cern.zoom.us/j/61522320218?pwd=ZGpWT3F6YXk0ZmRYT1dFTSswRkpmQT09, Aula 2.3*	*Frank-Dieter Gaede et al.* 14:30 - 14:40
Task 12.2 Turnkey Software	*https://cern.zoom.us/j/61522320218?pwd=ZGpWT3F6YXk0ZmRYT1dFTSswRkpmQT09, Aula 2.3*	*Andre Sailer et al.* 14:40 - 15:10
Task 12.3 Simulation	*https://cern.zoom.us/j/61522320218?pwd=ZGpWT3F6YXk0ZmRYT1dFTSswRkpmQT09, Aula 2.3*	*Anna Zaborowska et al.* 15:10 - 15:40
Coffee Break	*https://cern.zoom.us/j/61522320218?pwd=ZGpWT3F6YXk0ZmRYT1dFTSswRkpmQT09, Aula 2.3*	15:40 - 16:10
Task 12.4 Tracking	*https://cern.zoom.us/j/61522320218?pwd=ZGpWT3F6YXk0ZmRYT1dFTSswRkpmQT09, Aula 2.3*	*Hadrien GRASLAND* 16:10 - 16:40
Task 12.5 Particle Flow	*https://cern.zoom.us/j/61522320218?pwd=ZGpWT3F6YXk0ZmRYT1dFTSswRkpmQT09, Aula 2.3*	*John James Back* 16:40 - 17:10
Discussion and Wrap-up	*https://cern.zoom.us/j/61522320218?pwd=ZGpWT3F6YXk0ZmRYT1dFTSswRkpmQT09, Aula 2.3*	17:10 - 17:30

Task 12.2 Turnkey Software

turnkey software stack for all future collider projects

- take existing tools where possible - reuse existing software from the shared iLCSoft developed by ILC and CLIC
- all major players involved: CEPC, CLIC, FCC, ILC, EIC
- provide a complete data processing framework
  - shared components reduce overhead for all users
- make things as easy to use as possible for everybody (librarians, developers, users)
- supported by HSF, CERN EP R&D and **AIDAinnova**





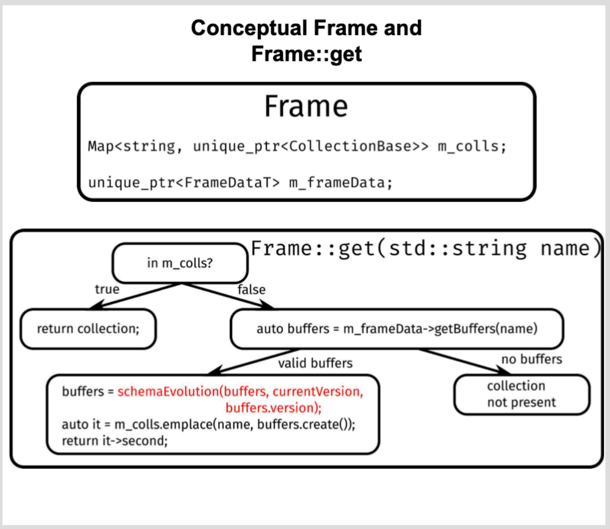
Task 12.2 Turnkey Software

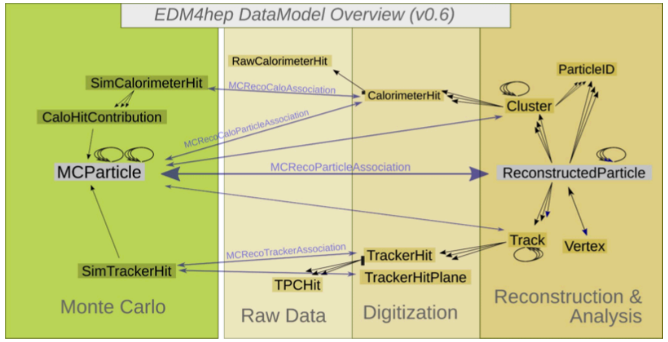
PODIO

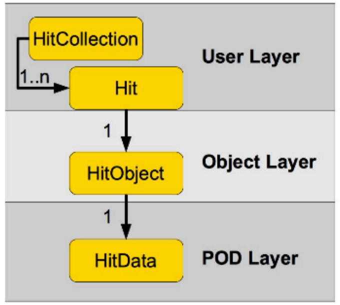
The event data model toolkit

- Generate code from simple yaml definition of EDM
- Based on using and storing POD (plain old data) structures
- Make it possible to target different I/O backends

✅ **Frame** class and concept (with accompanying multithreading model)
✅ License change to Apache2
✅ Allow datamodel extensions
✅ Generate code for dumping collections to JSON
✅ Many many changes under the hood
👷 **Schema evolution** of generated EDMs
👷 **Version 1.0** (backwards compatibility from then on)
👷 RNTuple based backend (try to merge podio#395 during hackathon)
👷 Some prototyping and testing on heterogeneous resources
👷 Small(-ish) additional features (already a few on the wish list)







✅ Addition of datatypes for drift chamber study
✅ Tool for dumping to JSON for Phoenix event display
✅ Used as “proper” upstream for EICD
👷 **Version 1.0** (backwards compatibility from then on, **needs PODIO schema evolution**)
👷 (Standalone) conversion from LCIO
👷 Utility functionality as necessary

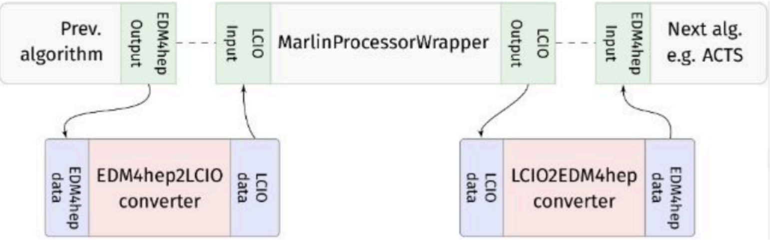
- lots of progress in PODIO/EDM4hep
- mostly re-design under the hood (Frames) and extension of data model (CEPC, EIC)
  - **schema evolution** under way !

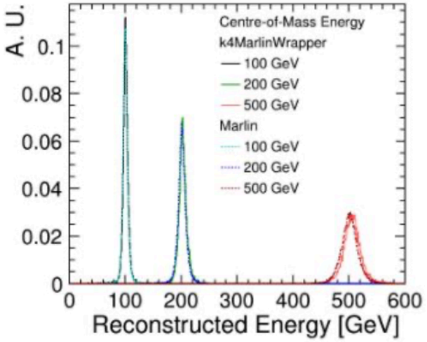
Task 12.2 Turnkey Software

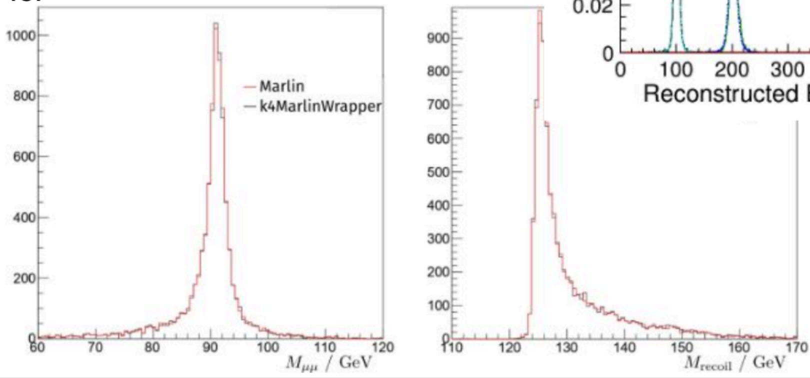
MS 47

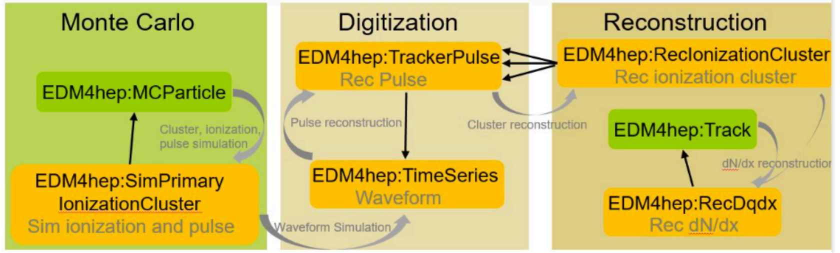
LC reconstruction prototype in Key4hep

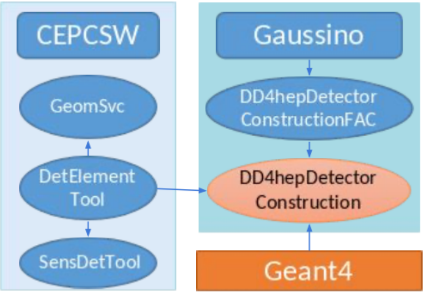
- Run unchanged Marlin Processors via Wrapper
- Configurable on-demand conversion between LCIO and EDM4hep (and vice versa)
- Steering file conversion script
- Extended testing uncovered a few smaller issues
- Excellent agreement between Marlin and Gaudi
- CLIC reconstruction run as part of CI for k4MarlinWrapper
- Working horse for k4CLUE studies
- Report online Jan 19, 2023

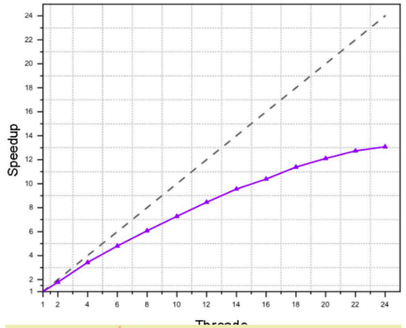


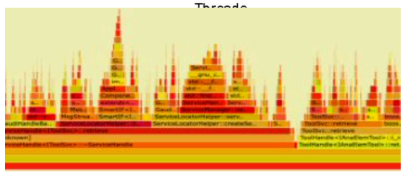












- MS47 running complete reconstruction for linear collider in Key4hep
  - using the MarlinWrapper (and iLCSoft part of Key4hep)

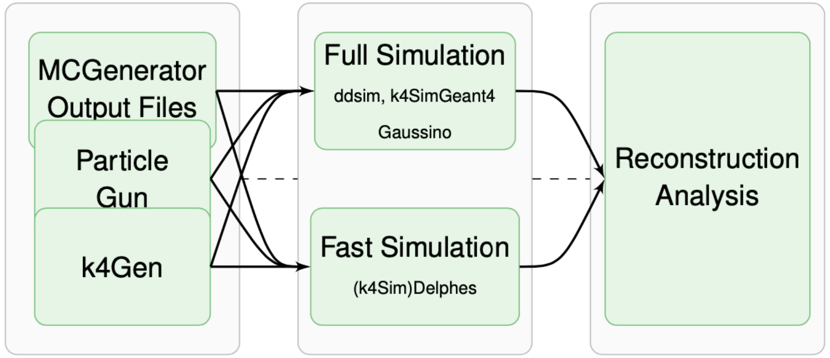
valuable contributions from associated
partners (IHEP, SDU) in context of using Key4hep for CEPC
- tracking, simulation, benchmarking, …

Task 12.2 Turnkey Software

This project has received funding from the European Union's Horizon 2020 Research and Innovation programme under GA no 101004761.

DD4hep Geometry and Simulations

- The simulations can be run in a stand-alone mode using the output from a Generator as input
- Work to integrate LHCb's Gaussino to replace framework integration on going (Graeme Stewart)
  - Ideally re-use existing components from DDG4, k4SimGeant4
- In all cases, the following step of (high level) reconstruction or analysis should be usable in the same way
- Moved lcgeo Github repository to key4hep/k4Geo, waiting for migration of FCCDetectors



significant activity at CERN for Key4hep

- simulation
- reconstruction (tracking/ACTS)
- framework (Gaudi)
- infrastructure (cvmfs, spack,…)
- …

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Reconstruction Developments

- Implement track fitting with ACTS, different fitting approaches (Gaussian Sum Filter), especially in view of electron reconstruction (Leonhard Reichenbach)
  - Apply for CLD tracking and detector optimisation studies
  - Integrate track reconstruction monitoring into validation framework
- Developments around Particle Flow Clustering and Pandora (Swathi Sassikumar)
  - Implement *DDGaudiPandora* interface between DD4hep Geometry and Pandora in the Gaudi framework, successor for *DDMarlinPandora*
  - Integrate Jet Energy Reconstruction monitoring into validation framework
  - Continue development to apply Pandora Clustering for LAr Calorimeter (IDEA-LAr, GranuLAr)
- Integration of k4CLUE (Erica Brondolin)

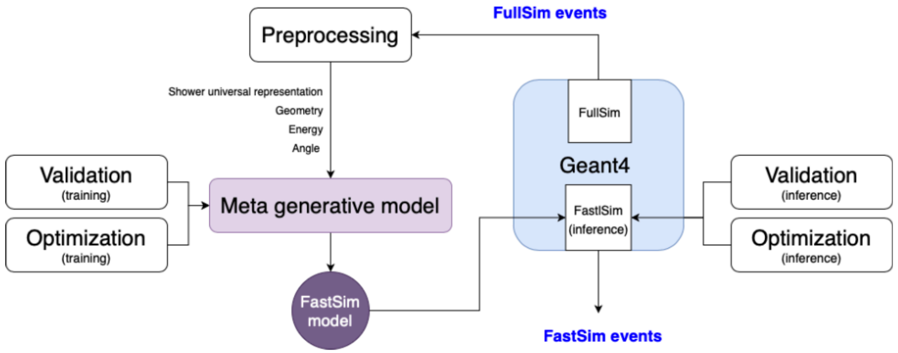
Task 12.3 Fast Simulation

Integration of ML models

Integration of Machine Learning (ML) models into standard simulation toolkit (GEANT4)

- Demonstration of ML inference in C++ framework
- available in GEANT4 11.0 release, but can be also used with 10.7
- Incorporation of few libraries: ONNX Runtime, LWTNN, Torch
  - Torch was integrated during the last AIDAinnova hackathon, thanks to everyone involved! (CERN, DESY, UniMan)
  - available in GEANT4 11.1 release
- Implemented as a Geant4 example Par04, includes a trained model: Variational Autoencoder (VAE)
- Described in AIDAinnova milestone report

MS 49



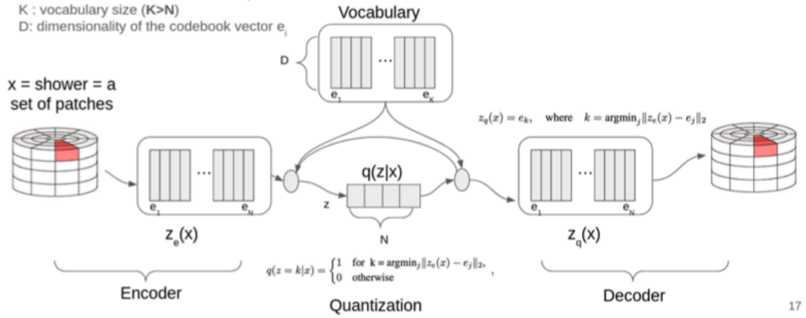
MS49: runnable prototype of ML fast sim in Geant4
provides basis for eventually including results from AIDAinnova 12.3 in real physics simulations

Development of new ML model

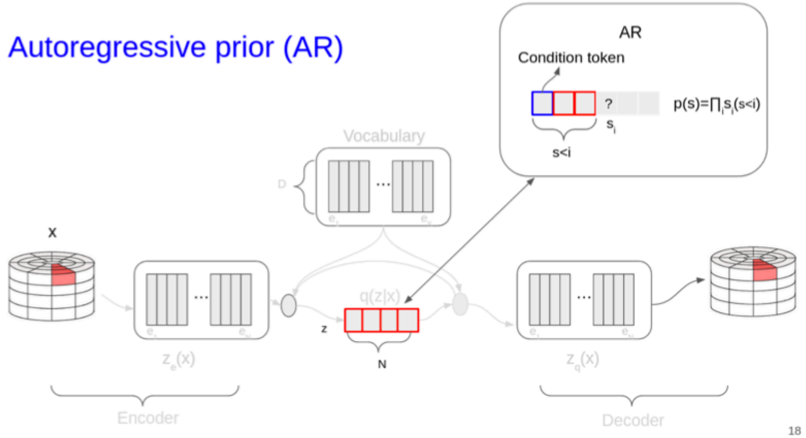
VQ-VAE

- VQ-VAE was first introduced in the "Neural Discrete Representation Learning" paper in 2017 by DeepMind
- It is a combination of a variational autoencoder (to learn lower representation of the input data) and then discretizes this representation using a vector quantization step to map it to a finite set of discrete codes

- z: discrete latent variable
- Latent embedding space e ε R^{NxD}
- N: number of codebook vectors to represent a shower
- K : vocabulary size (K>N)
- D: dimensionality of the codebook vector e_i

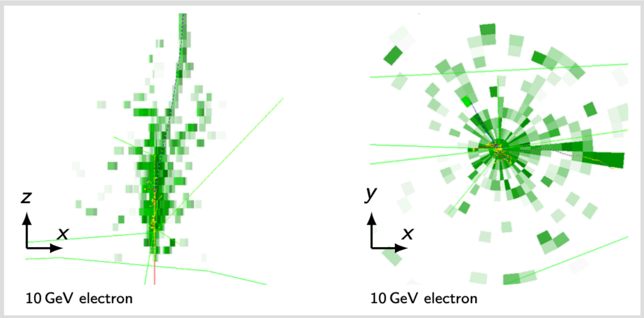


Autoregressive prior (AR)



- at CERN started to investigate new types of ML models: transformer
- collaboration with IBM

Task 12.3 Fast Simulation

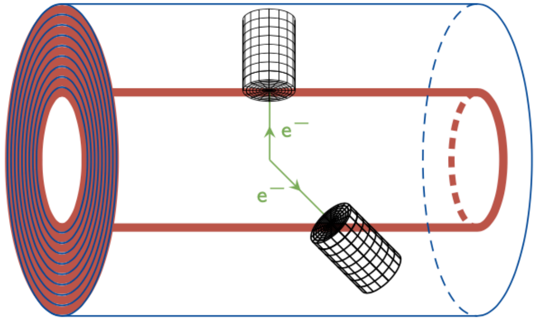


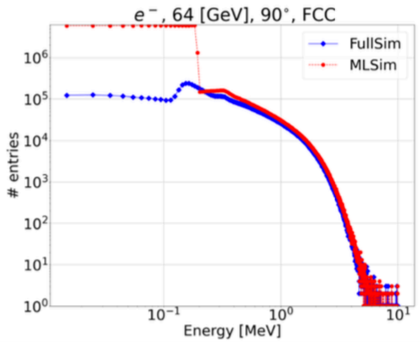
MetaHEP

MetaHEP shows how meta-learning can aid application of ML models for fast shower simulation.

- Shifts focus from development of custom ML models tied to detector readout to integration of energy deposition from a regular grid to the detector readout.
- Existing VAE model produces good results for almost all shower observables, but cell energy distribution remains a challenge (blurry images) → this model may not be accurate for high granularity calorimeters
- Work presented at ACAT 2022

Training	Steps	Convergence time
Traditional	400	20 min
Traditional	3900	3h 15min
Adaptation	400	20.5 s
527 speed-up		





- MetaHEP provides possibility to very quickly train/adapt ML fast sim models to a new calorimeter
- potentially optimal solution for coarser calorimeters and quick studies

Lamarr and the Gudi functional framework

What and why

- Currently work to implement the Gaudi Functional Framework (GFF) into Lamarro
- Motivation for using GFF
  - Take advantage of its native multithreading
  - Modernization of the Code

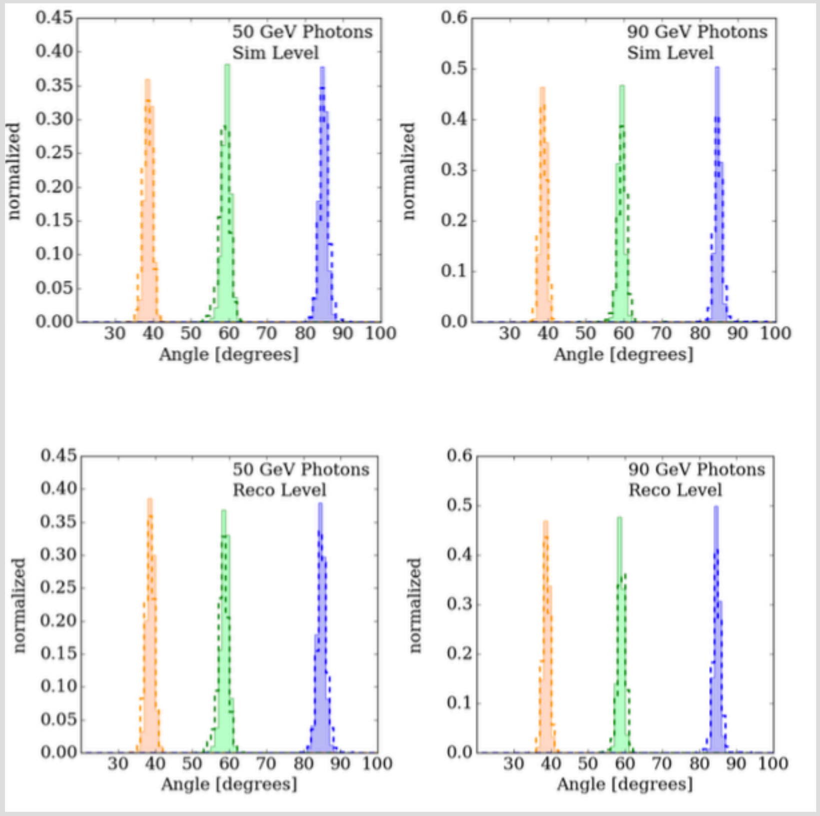
Progress

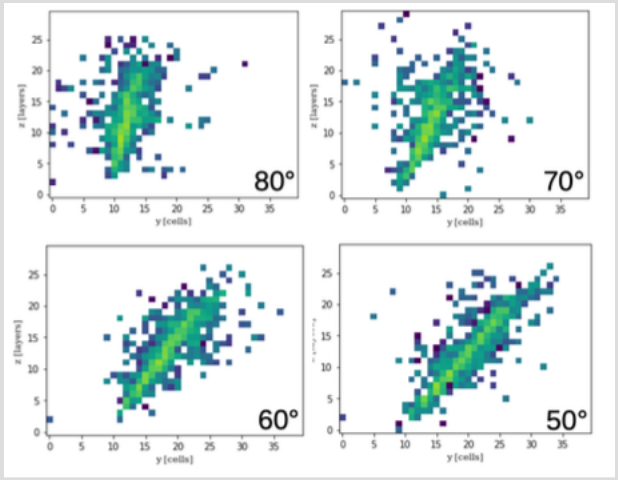
- Majority of the calorimeter has now been ported over to GFF
- Had some issues with importing geometry in a thread safe manor
  - This has been addressed
- Still having issues with thread safety of random number generator which needs to be addressed
  - Work on going
- Branch LamarrGaudi

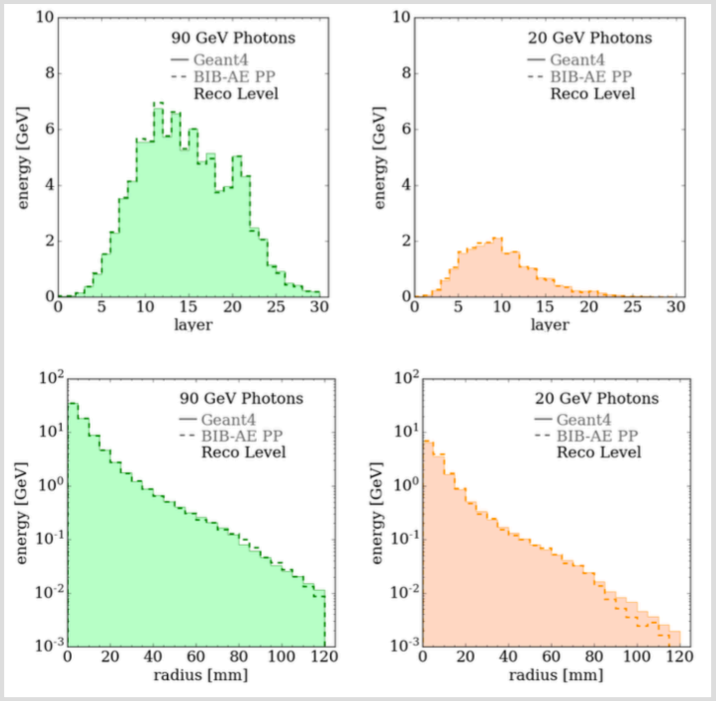
work on porting Lamar fast sim from LHCb to Key4hep started at UMan

Task 12.3 Fast Simulation

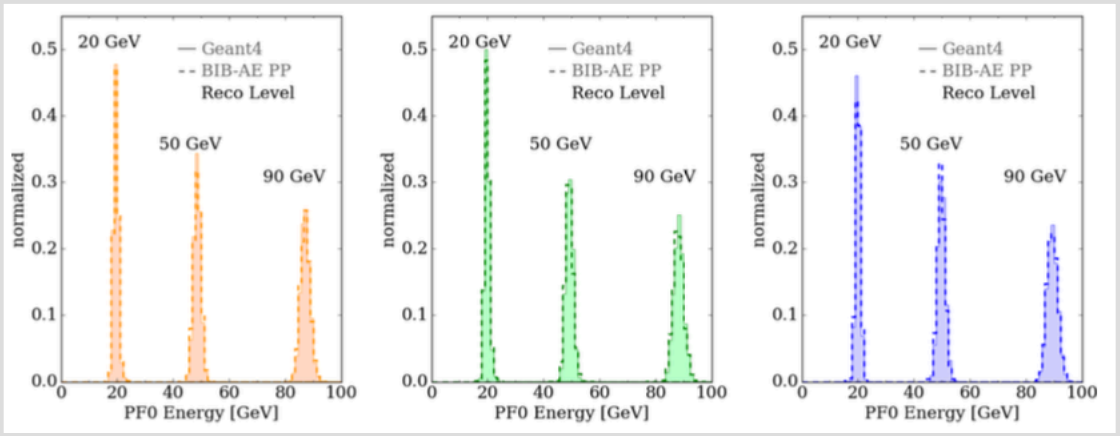
Angular and Energy Conditioning







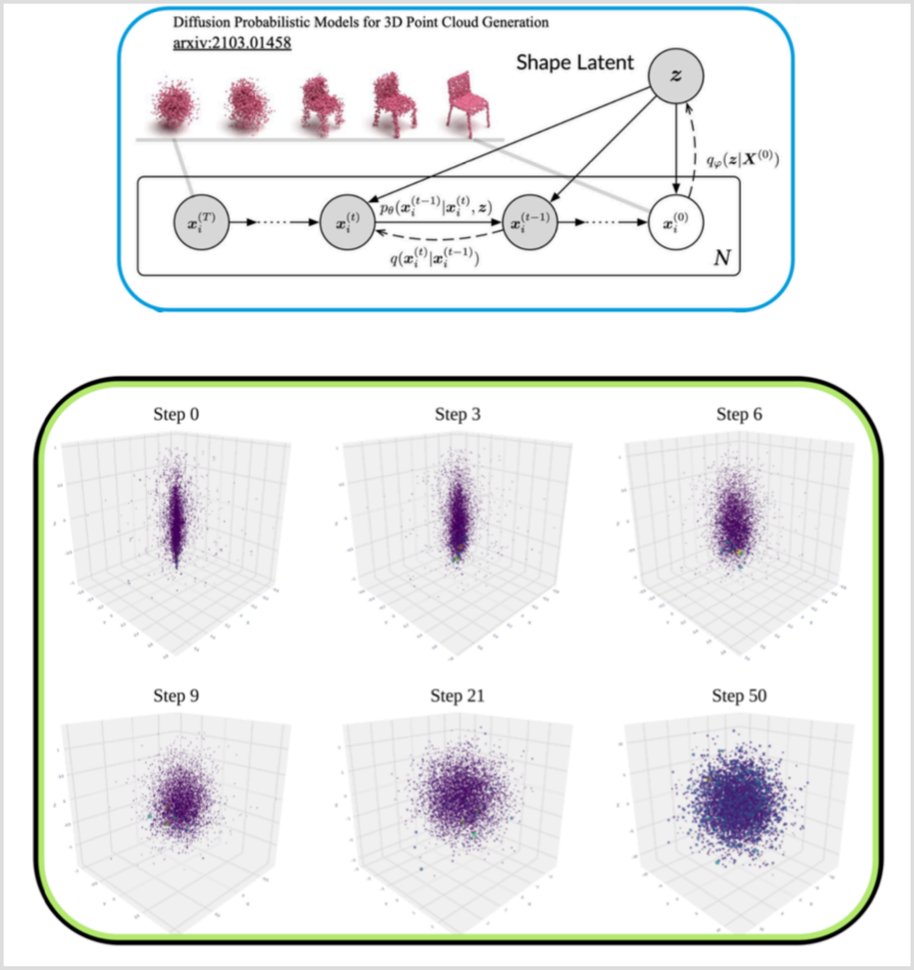
New Angles on Fast Calorimeter Shower Simulation, S.Diefenbacher, P.McKeown et al arXiv: 2303.18150, submitted to MLST

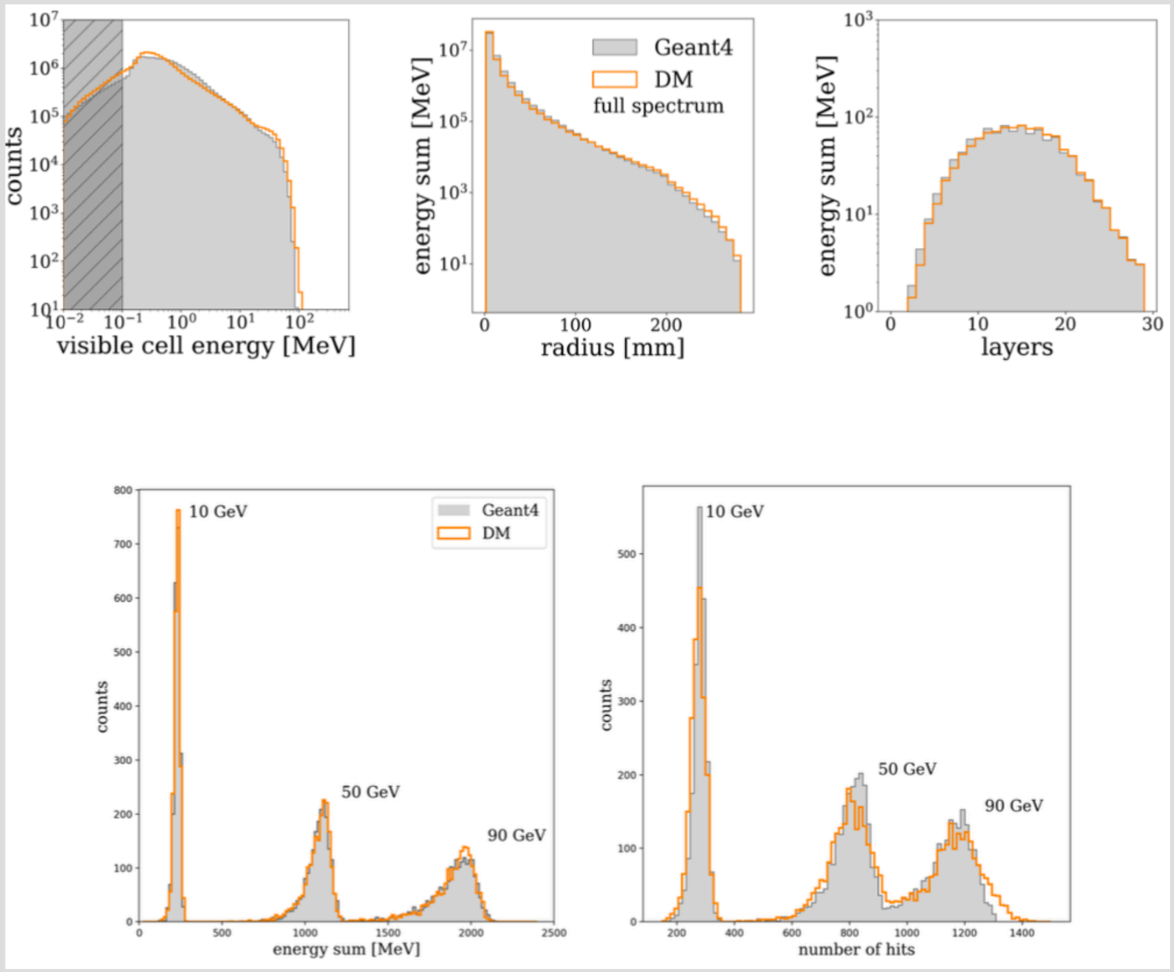


- achieved very high physics fidelity for fast simulation with BIB-AE conditioned on energy and impact angle
- necessary for realistic calorimeter simulations

Task 12.3 Fast Simulation

Difusion Point Clouds



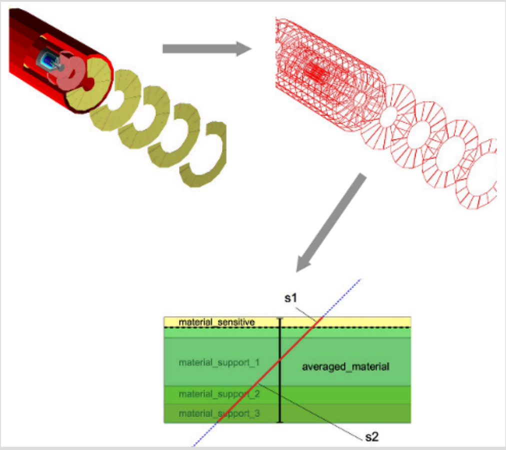


- achieved good fidelity with a point cloud diffusion model using ultra-high granularity
  - should solve issue with realistic detector geometry

Task 12.4 Track Reconstruction

Main work in track reconstruction task is framed inside the ACTS project

- A Common Tracking Software
- Project was spawned from ATLAS's tracking code
- Make this state-of-the-art track reconstruction experiment independent
  - Significant technical challenges!



Acts core : Geometry

- Removed need for ActsExtension in DD4hep detectors
- SVG geometry display (shared with detray)
- Ongoing work towards detray-like layerless geometry in Acts
- Lots of work on Geant4 bugs, including better GDML import

Acts core : I/O and event data

- Generic MultiTrajectory storage (for e.g. xAOD integration)
- EDM4hep support introduced, improved in #2001 #2022
- More memory-efficient measurement storage
- Ongoing work on public Track EDM

- good progress on integrating ACTS into Key4hep framework - DD4hep geometry and EDM4hep
  - more work needed soon (also w/ ACTS experts not in AIDAinnova)

Task 12.4 Track Reconstruction

Acts core : Track finding & fitting

- Gaussian Sum Filter integrated, refined throughout the year
- Exa.TrkX ML track finding integrated, CI'd, being modularized
- Global χ^2 fitter integrated

Acts core : Infrastructure, misc

- GPU CI for Acts, vecmem, detray, traccc
- Ambiguity resolver integrated, optimized
- Test Athena build on every main branch commit
- Early C++20 support, primary CI target is now Ubuntu 22.04
- Tests of public headers in algebra-plugins, vecmem

R&D : algebra-plugins

- Used GSoC to investigate alternatives to Eigen
  - Fastor proved most interesting (~3x faster in µ-benches)
  - Was recently integrated, enables more realistic benches

R&D : traccc

- CUDA : FastSV clustering, (C)KF from Berkeley*
- SYCL : clustering, seed finding
- Continued effort on on making these share code, e.g. #377
- Evaluating various other options : Futhark, Kokkos, Alpaka…
- Optimizations : faster kernels, alloc reuse, async memcpy…
  - Recent highlight : reworked EDM → 60 % speedup
- Recently got proper CPU benchmarks, enabling comparisons

- significant development on ACTS 'under the hood'
  - better and faster algorithms, linear algebra, parallelisation, code optimisation…

Task 12.4 Track Reconstruction

Machine Learning for (resistive) MPGDs

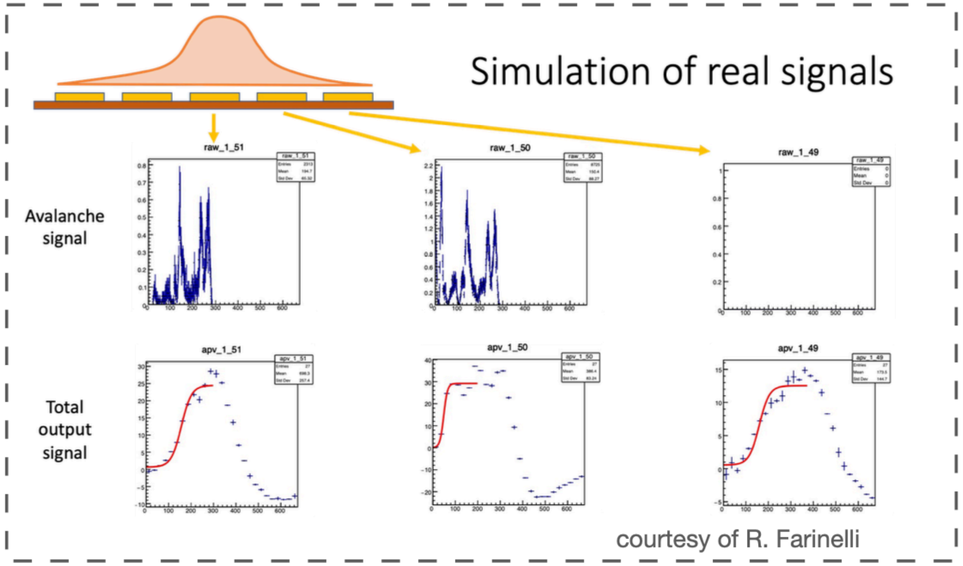
The task in a nutshell

- Goal: use M.L. algorithms to improve tracking performance and PID capability to (resistive) MPGDs
  - Possible application pre-shower of the IDEA detector at FCC_{ee}

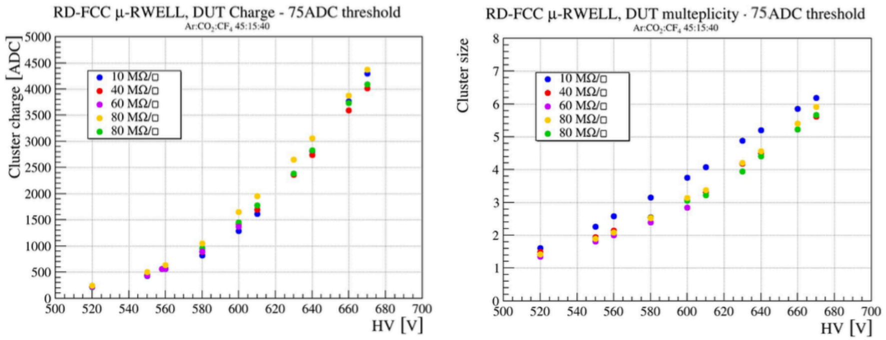
Aidainnova 4-year program

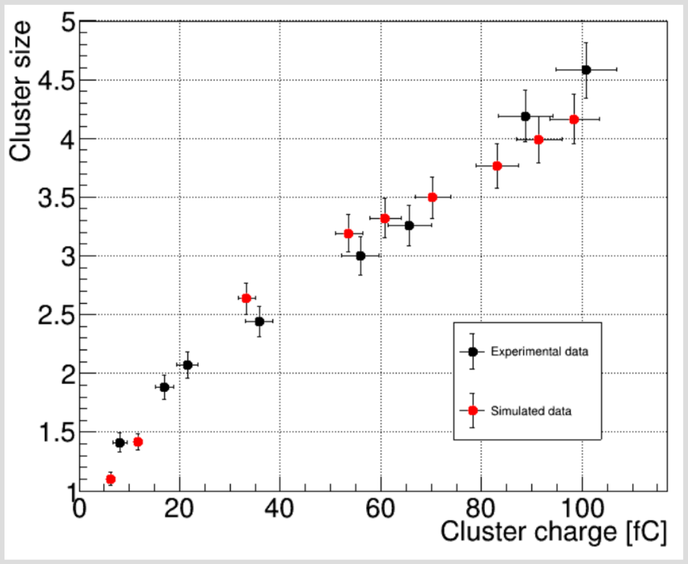
1. simulation of the μ-RWELL resistive layer
2. use of Machine Learning for cluster selection and track finding
3. track cleaning and refinement
4. application to IDEA framework

- Groups involved: INFN Bologna, Ferrara, Frascati and Turin
- Strong interplay with tasks
  - **7.3** design and industrialization of large area microRWELL detectors (we receive input from there)
  - **11.2** design of an ASIC chip dedicated to microRWELL readout (input from our simulations)
- Synergy with Eurizon European project



test beam data





Task 12.4 Track Reconstruction

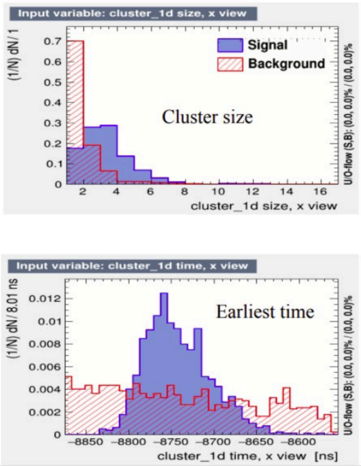
Machine Learning for (resistive) MPGDs

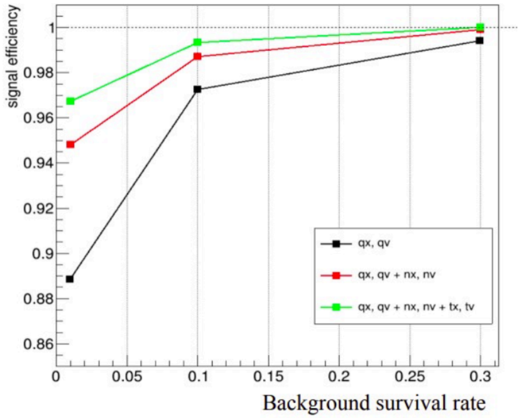
Aidainnova 4-year program

1. simulation of the μ-RWELL resistive layer
2. use of Machine Learning for cluster selection and track finding
3. track cleaning and refinement
4. application to IDEA framework

- Machine Learning to separate signal from noise at hit/cluster level (classification)
- Use TMVA, Boosted Decision Tree

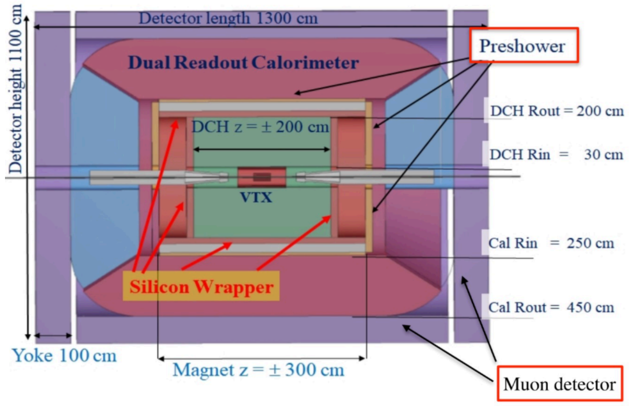
  cluster 1d Charge x, v + cluster 1d size x, y + fastest hit in cluster 1d x, y





- Complete Test Beam data analysis (in progress) ➡ **DONE**
- Perform Simulation Tuning with TB data (fall 2022) ➡ **DONE**
- Develop cluster reconstruction algorithms based on detector simulation (2022-23) ➡ **IN PROGRESS**

next step: apply ML reconstruction to IDEA detector for FCCee



Task 12.5 Particle Flow Reconstruction

Particle Flow Algorithms (PFAs)
State-of-the-art reconstruction for HEP calorimeters and neutrino detectors

Research Groups (main contacts)

- **Dual Readout Calorimeters**:
  - I. Vivarelli (Sussex), B. Di Micco (INFN Roma-3), S. Vallecorsa (CERN)
- **APRIL, Algorithm for Particle Reconstruction @ ILC**:
  - G. Grenier (CNRS-IP2I), V. Boudry (CNRS-LLR)
- **DUNE Near Detector reconstruction**:
  - J. Marshall* & J. Back* (Warwick), M. Uchida & S. Dennis (Cambridge)

* WP12.5 co-conveners

- goal: develop sophisticated PFA algorithms
- for a variety of new detectors

integrate everything in PandoraSDK (and thereby in **Key4hep**)

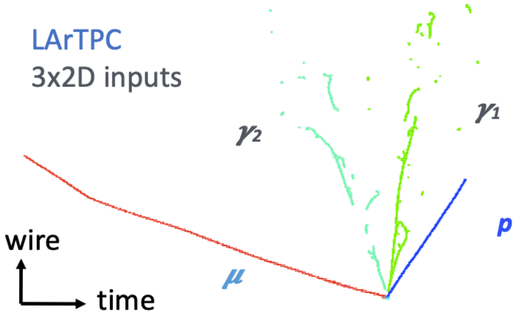
Pandora Software Development Kit

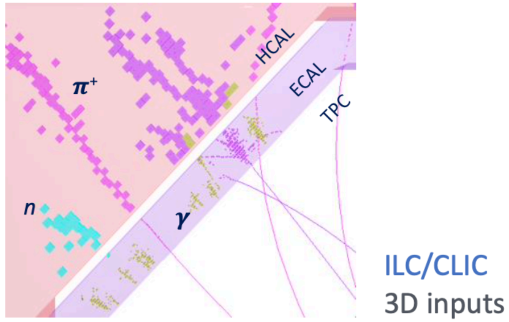
https://github.com/PandoraPFA

A single clustering approach is unlikely to work for complex event topologies:

- Mix of track-like & shower-like clusters

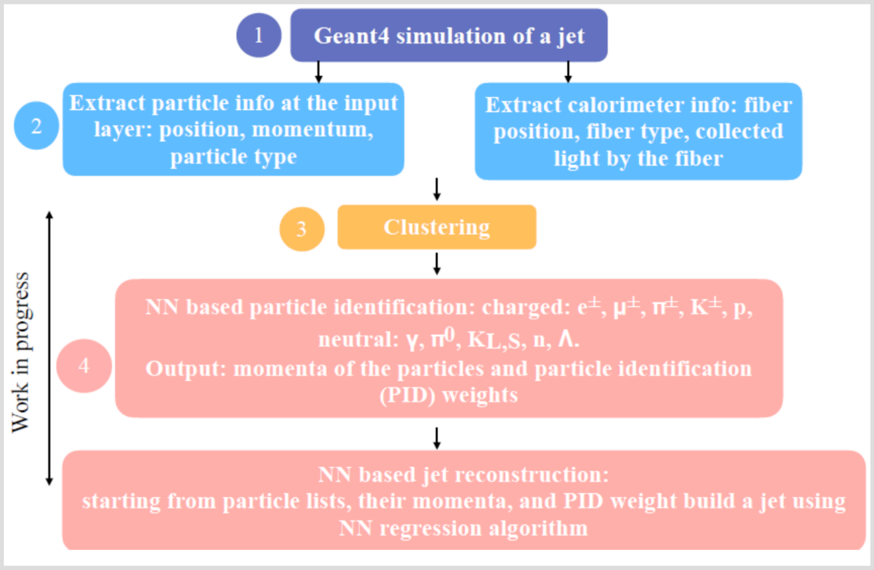
- Use **multi-algorithm** approach using the **Pandora SDK** to **build up events** gradually:
  - Each step is **incremental** - aim not to make mistakes (undoing mistakes is hard)
  - Deploy **more** sophisticated **algorithms** as picture of **event develops**
  - Algorithms: can use machine-learning methods & detector physics knowledge

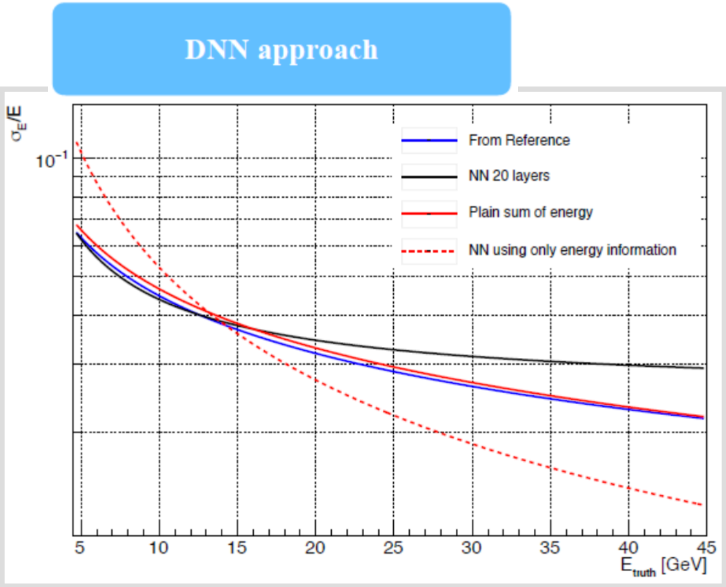


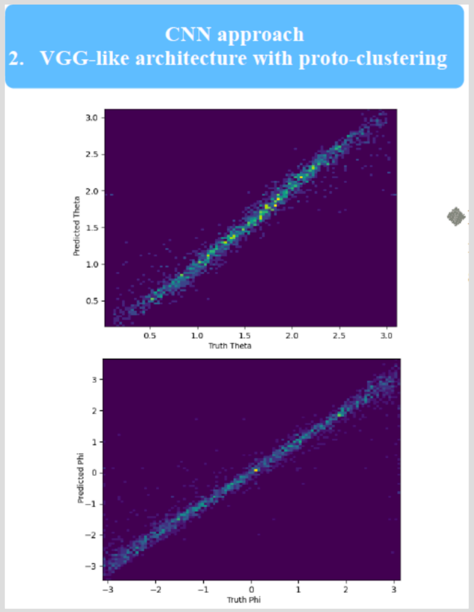


Task 12.5 Particle Flow Reconstruction

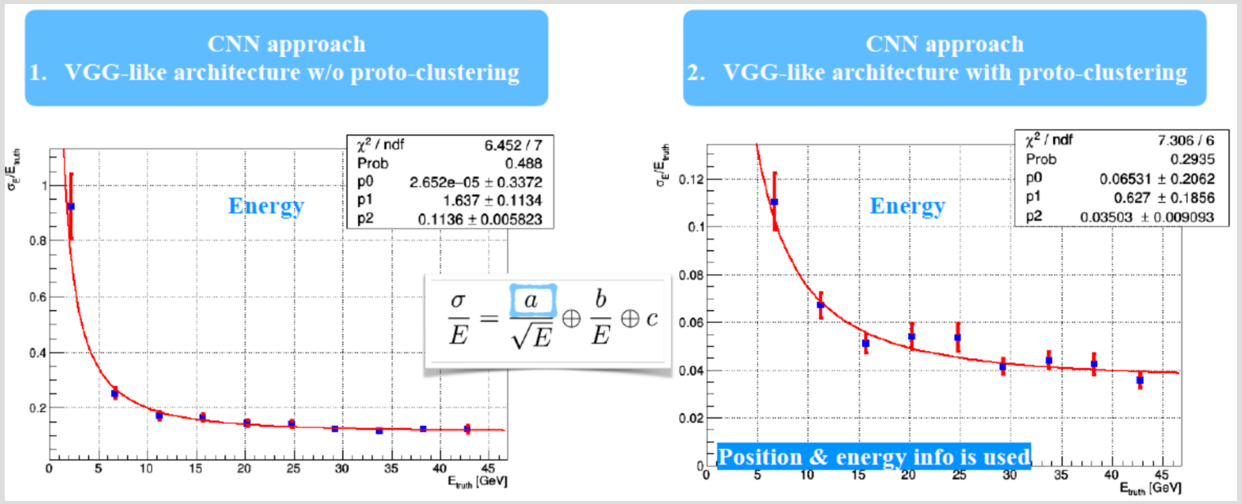
PFA for Dual Readout Calorimeter







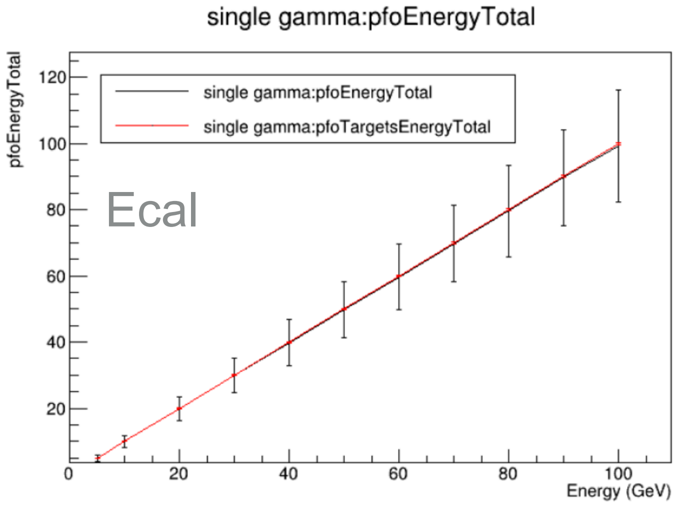
electron reconstruction w/ DNN and CNN



goal: develop ML algorithms **for full jet reconstruction**
with **optimal Jet Energy Resolution**
for a dual readout calorimeter

Task 12.5 Particle Flow Reconstruction

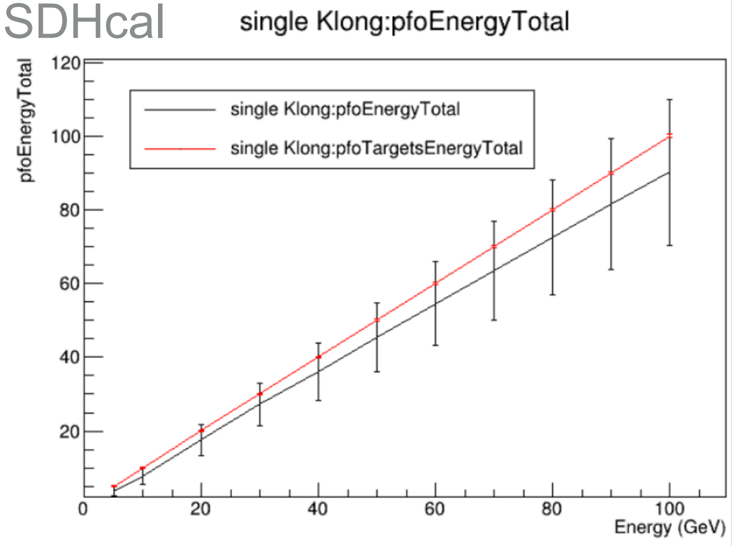
APRIL: Algorithm for Particle Reconstruction at the ILC



Pandora calibration for ILD option 2

1) Calibration for SDHCAL : doesn't look that good but closest inspection shows
   1) Endcap is OK (see next slide)
   2) Barrel is too low (see next slide)
2) **SDHCAL is correctly calibrated but it lacks a correction** to correct cluster energy depending on the incidence angle of the cluster particles.
3) In the left plot, error bars represents the width of the energy distribution for single klongs.
4) Next step : implement angle correction.

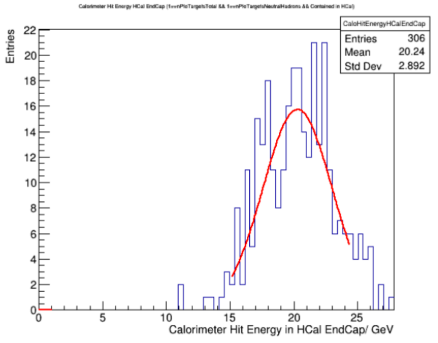
SDHcal



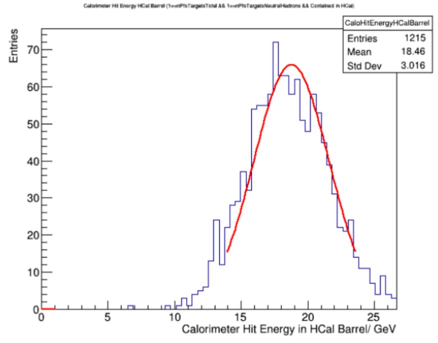
goal: develop particle flow reconstruction in PandoraSDK addressing ILD w/ SDHcal option

working on angular correction of energy calibration in SDHcal …

1) Particles fly perpendicularly to layer surfaces.



1) Particles do not fly perpendicularly to layer surfaces.



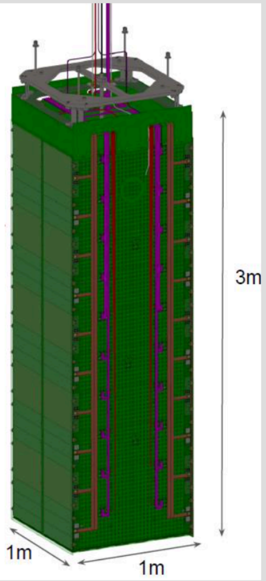
Task 12.5 Particle Flow Reconstruction

Dune Near Detector Reconstruction

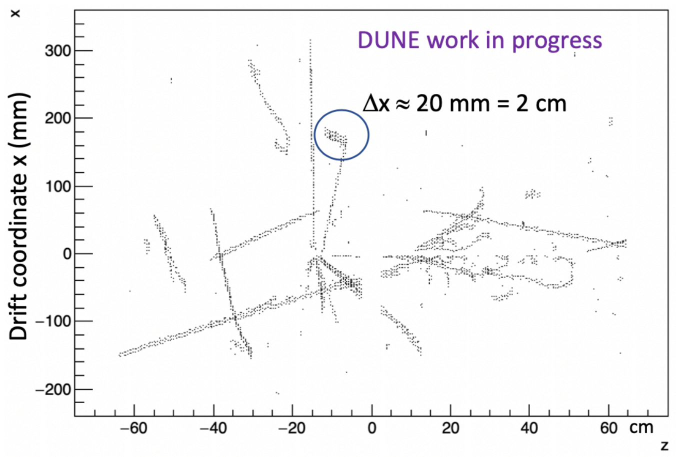
- ND LAr = 7x5 array of 1x1x3 m^3 modules, optically segmented LAr TPCs, 3D pixel readout
- 2x2 prototype: data taking during 2023

- Using **Pandora** for reconstructing 2x2 data
- "2x2 simulation challenge" underway
  - Centrally produced multi-neutrino events
  - larnd-sim digitisation applied to Geant4 (edep-sim) hits
  - HDF5 format; decoded for Pandora input

- Expect ~50 ν interactions per sec for 7x5 ND LAr
  - LBNF 120 GeV, 1.2 MW proton beam on graphite target
  - Secondary $\pi \rightarrow \mu\nu$: 7.5x10^{13} protons per beam "spill" (1.2 sec)

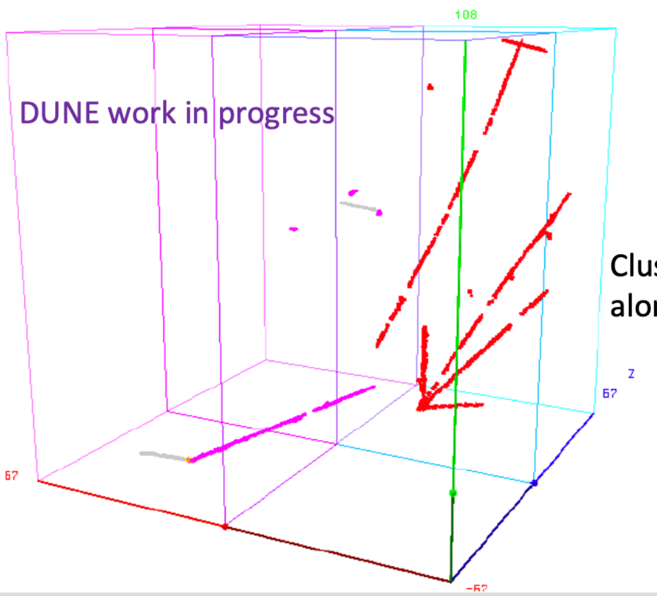


2D projection



Tracks appear "fuzzy": few cm spread of hits along drift x
Caused by charge deposition affecting neighbouring pixels

"3D" ND Reconstruction

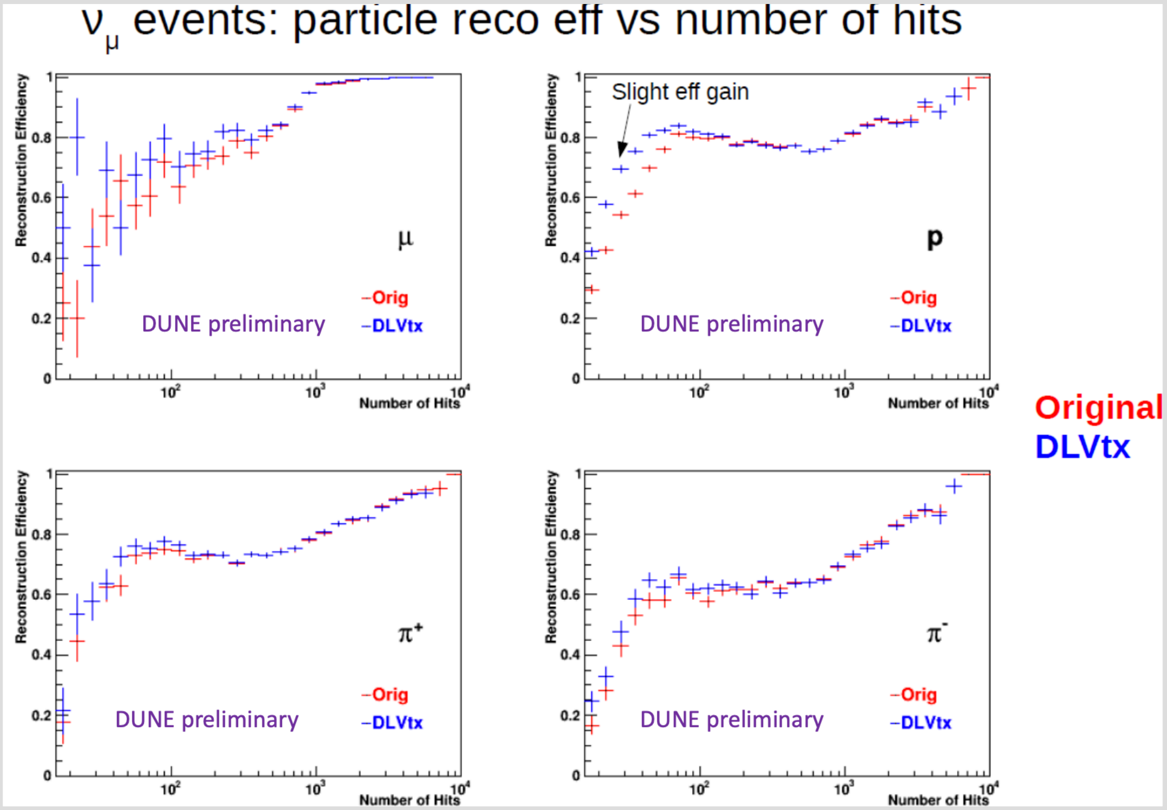


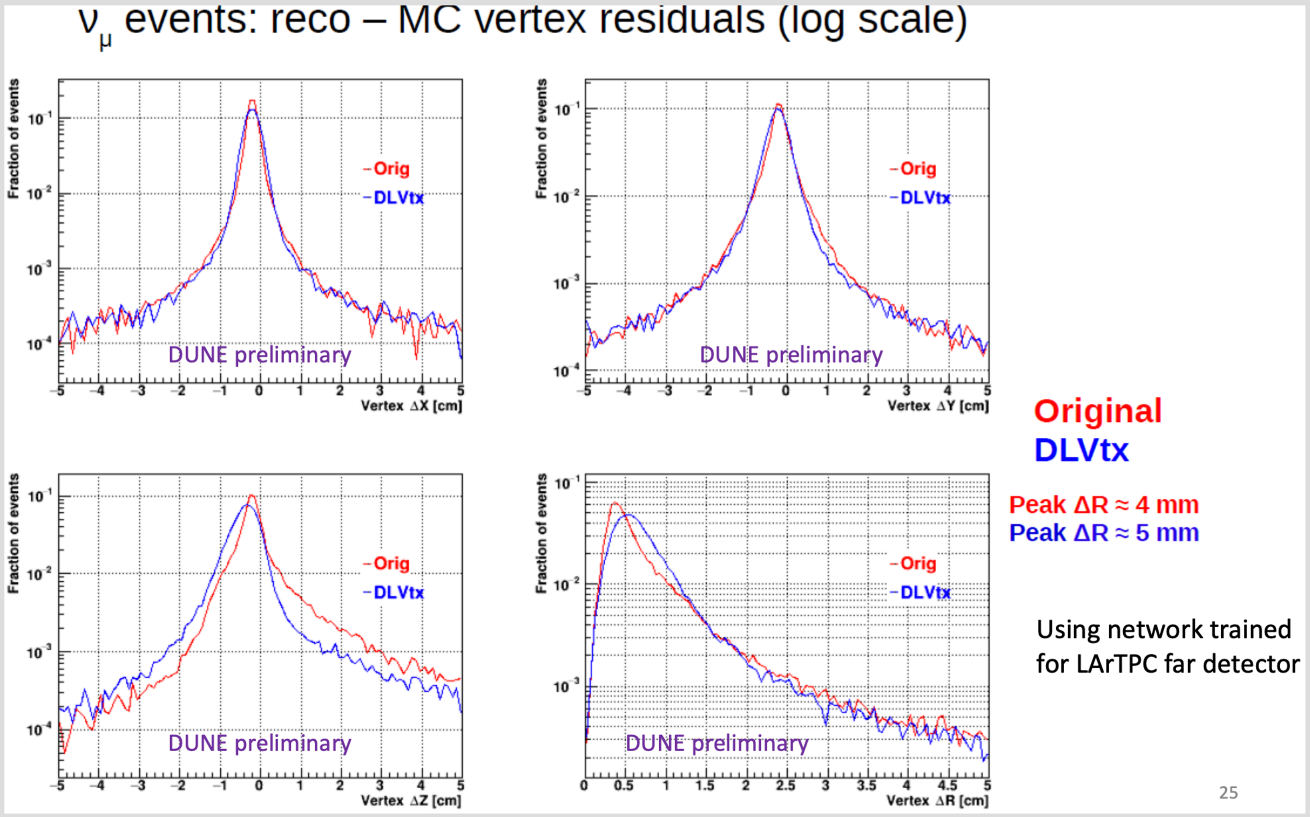
Clusters overlap along y projection

- developed Near Detector reconstruction for 2x2 simulation challenge and data taking
- working on optimising 3D reconstruction

Task 12.5 Particle Flow Reconstruction

Dune Near Detector Reconstruction





- started work on Deep Learning (DL) vertexing for Near Detector with DL from Far Detector
- need dedicated re-training …

WP12 Hackathon

in Valencia 2023

- used opportunity of having many software experts in one place to have the **2nd edition of the AIDAinnova WP12 hackathon**
- addressed many open issues and challenges:
  - closed many longstanding issues in Key4hep Github
  - created a **Key4hep stack** with latest tools and developments - including ML inference libraries for fast simulation
  - investigated **ML inference** with different network architectures, inference libraries
    - comparison of CPU vs GPU
  - discussions on general strategy and next steps …

```cpp
/// User callback to model the particle/energy shower - details defined in ML_MODEL
virtual void modelShower(const G4FastTrack& track, G4FastStep& step) override {

  // remove particle from further processing by G4
  step.KillPrimaryTrack();
  step.SetPrimaryTrackPathLength(0.0);
  G4double energy = track.GetPrimaryTrack()->GetKineticEnergy();
  step.SetTotalEnergyDeposited(energy);


  _input.clear() ;
  _output.clear() ;
  for( auto& layerSPs : _spacepoints )
    layerSPs.clear() ;

  fastsimML.model.prepareInput( track, _input , _output ) ;

  fastsimML.inference.runInference(_input, _output ) ;

  fastsimML.model.convertOutput( track, _output , _spacepoints) ;

  fastsimML.geometry.localToGlobal( track, _spacepoints ) ;

  // now deposit energies in the detector using calculated global positions

  for( auto& layerSPs : _spacepoints )
    for( auto& sp : layerSPs ) {
      fastsimML.hitMaker->make( G4FastHit( G4ThreeVector(sp.X,sp.Y,sp.Z) , sp.E ), track);
    }
}
```

Conclusion

and outlook

- WP12 “Software for Future Colliders” very successful in first half of AIDAinnova

  - **met all Milestones on time**
  - **excellent progress in all tasks**

- final software stack with all new algorithms and tools seems within reach

  - identified a few loose ends and topics to be addressed in the next year(s)