Towards production readiness with the Key4hep software stack for future colliders

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for the Key4hep developers

LCWS 2024

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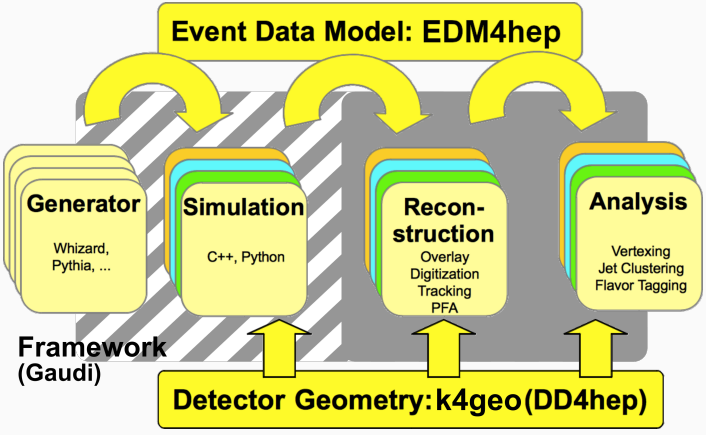
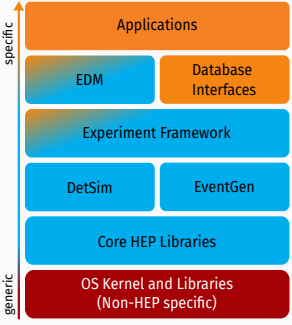
From generation to analysis - the general workflow



- Many steps involved from generating events to analyzing them
- Hundreds of SW packages
  - Building & deploying
  - Consistency
  - Reproducibility
- Try to give an overview of the **Key4hep** SW ecosystem
  - Highlight LC related parts

Key4hep - A (very) brief introduction

- Future detector studies rely on well maintained software for studying their potential
- Maintenance of a consistent HEP SW stack is non-trivial
  - Ecosystem of interacting components
- Sharing the burden allows everybody to reap the benefits
  - Make best use of scarce (human) resources
- **Regular contributions from ILC, CLIC, FCC, CEPC, EIC, (MuonCollider), ...**
- Support from major R&D initatives
  - CERN R&D for Future Experiments, AIDAinnova WP12, ECFA

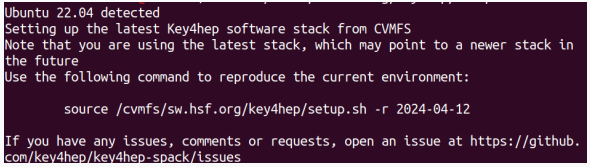


Keyhep releases and nightlies

- (Rolling) latest release of the complete Key4hep software stack
  - Full stacks for AlmaLinux9, Ubuntu22.04, (CentOS7)

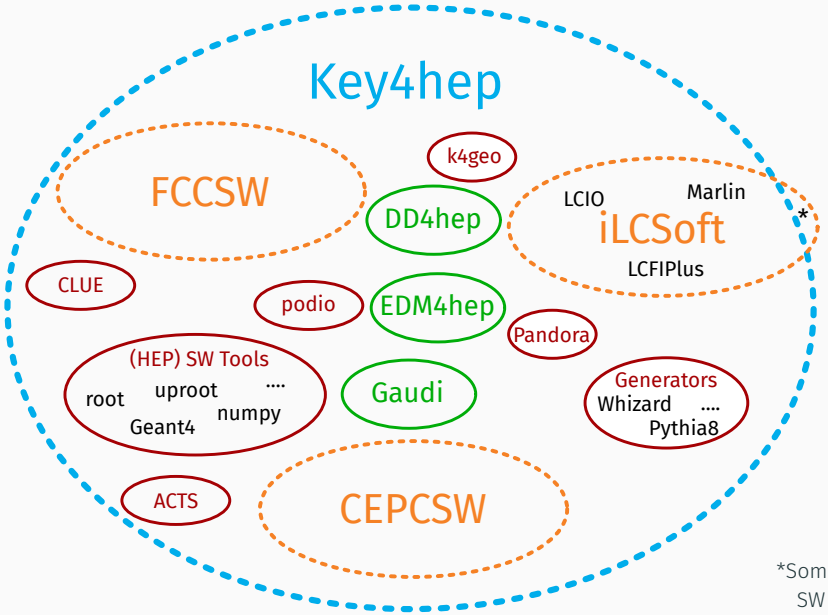
```
/cvmfs/sw.hsf.org/key4hep/setup.sh
/cvmfs/sw-nightlies.hsf.org/key4hep/setup.sh
```

- Documentation
  - key4hep.github.io/key4hep-doc
  - Includes tutorials & How-tos



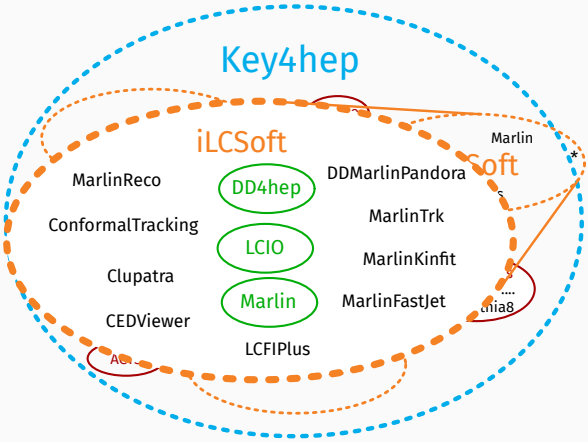
- **Release early and release often**
  - Make fixes available early
  - Discover problems and collect feedback as early as possible
- Biweekly, alternating meetings for Key4hep & EDM4hep
  - indico.cern.ch/category/11461/

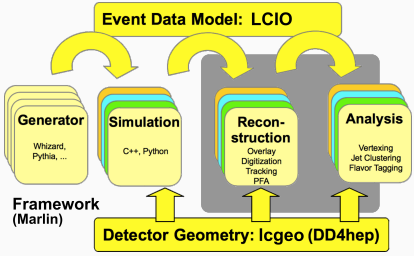
Key4hep (simplified) overview



*Some testbeam related SW not yet included

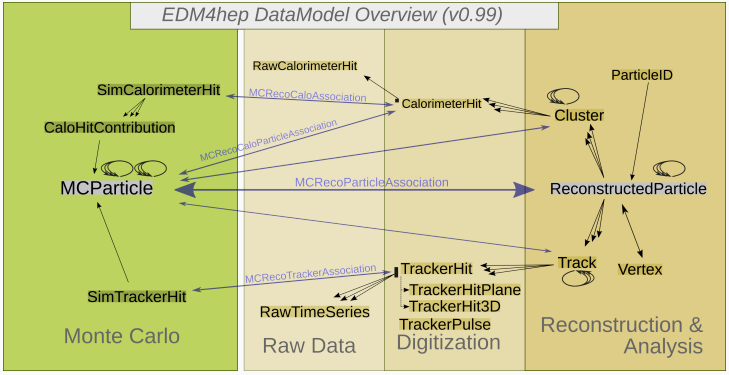
iLCSoft - The stack inside the stack





- Full suite of reconstruction & analysis tools
  - Used in numerous productions for LC studies
- LCIO vs EDM4hep
- Marlin vs Gaudi

EDM4hep - The common EDM for Key4hep

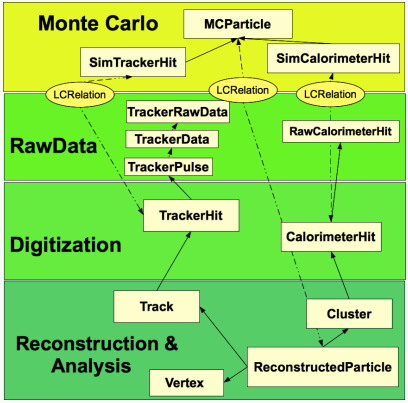


- Based on `LCIO` and `FCC-edm`
  - Focus on usability in reconstruction & analysis
- Currently finalizing v1.0
- Can easily be extended
  - Used by EDM4eic
  - Prototyping!
- Generated via `podio`
  - **v1.0 now available!** 🎉

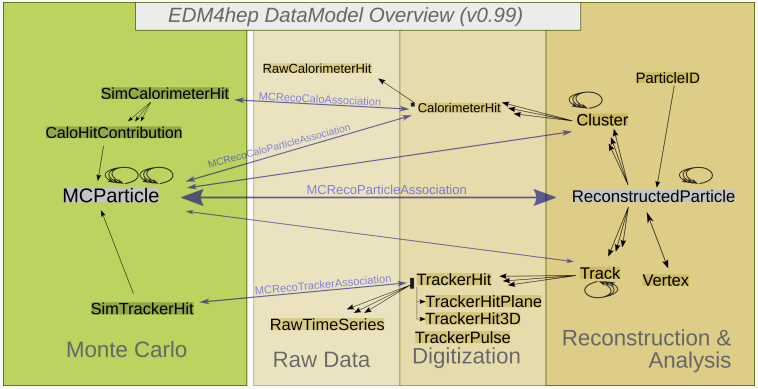
key4hep/EDM4hep
edm4hep.web.cern.ch
AIDASoft/podio
key4hep.web.cern.ch/podio

LCIO vs EDM4hep (at the highest level)

LCIO



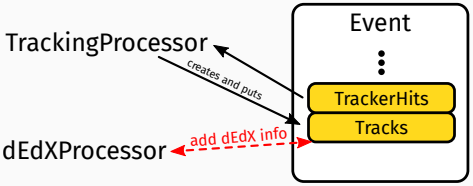
EDM4hep



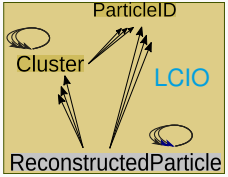
- Since EDM4hep is based on LCIO the high-level structure is very similar
- Some differences in philosophy and implementation
- **Conversion in both directions available in Key4hep** as a library

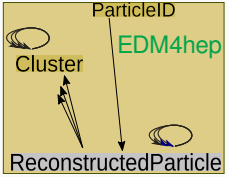
LCIO vs EDM4hep - The conceptual differences

- `LCRelations` vs `Associations`
  - LCIO: (in principle) arbitrary types
  - EDM4hep: dedicated associations only
- Mutability concept
  - LCIO: (almost) always
  - EDM4hep: only at creation time
- Revised some datatypes and their relations
  - `Track`, `Vertex`, `ReconstructedParticle`, `ParticleID`
- Ensure similar functionality with utilities
- Try to keep algorithms / processors as focused as possible



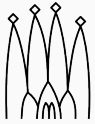

```
edm4hep::RecDqdx:
  Description: "dE/dx or dN/dx"
  Members:
    - edm4hep::Quantity dQdx  // value + error
  OneToOneRelations:
    - edm4hep::Track track    // computed from here
```





Experiment Framework & Core components

- `Gaudi`, originally developed by LHCb, now also used by ATLAS, FCCSW and smaller experiments
  - Supports concurrency
  - “Battle-proven” from data taking during LHC operations



- Key4hep has decided to adapt `Gaudi` as its experiment framework
  - Contribute to its development where necessary

The `k4FWCore` package

key4hep/k4FWCore

- Providing core functionality, e.g.
  - Data Service for EDM4hep / podio inputs
  - `k4run` for running options files
- Multithreading support via `Gaudi::Functional`
- Support for variable, runtime configurable number of inputs / outputs

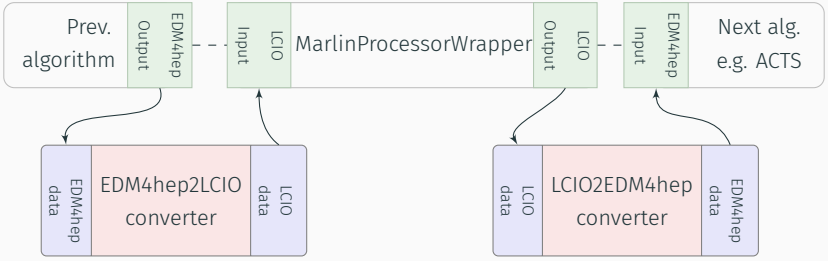
Marlin vs Gaudi

- Conceptually the two frameworks are very similar
  - Schedule different working units
  - Marshall data
- Most obvious differences in naming conventions
  - As always some differences emerge when looking at the details

	Marlin	Gaudi
language	C++	C++
working unit	Processor	Algorithm
config language	XML	Python
transient data format	LCIO	anything
set up function	`init`	`initialize`
work function	`processEvent`	`execute`
wrap up function	`end`	`finalize`

k4MarlinWrapper

- Wraps Marlin processor in a Gaudi algorithm and allows to run them unchanged
- Automatic, on-the-fly conversion between LCIO and EDM4hep
- Allows to “mix and match” existing reconstruction algorithms with new developments
  - Working horse for many FCC full simulation studies at the moment



ILD standard reconstruction in Key4hep

- All configuration available from iLCSoft/ILDConfig
- Everything that works in iLCSoft also works in Key4hep!

```
Marlin MarlinStdReco.xml --global.LCIOInputFiles=<input-file> [...]
```

- Now also with Gaudi

```
k4run ILDReconstruction.py --inputFiles=<input-file> [...]
```

  - Works with EDM4hep and LCIO inputs
  - EDM4hep output by default, LCIO output via `--lcioOutput=[true|only]`
- Facilitates collaboration with other projects, e.g. CLD
- Full migration of all workflows will take some time but process started
  - Some new developments already done exclusively in Gaudi configuration

iLCDirac - Using Key4hep in production

- iLCDirac provides functionality to run jobs on grid resources
- Extensively used for productions using iLCSoft
- Key4hep releases & nightlies available through iLCDirac
  - Similar to using `Marlin`

GaudiApp

Gaudi Application to run applications based on Gaudi.

New in version v32r0p1.

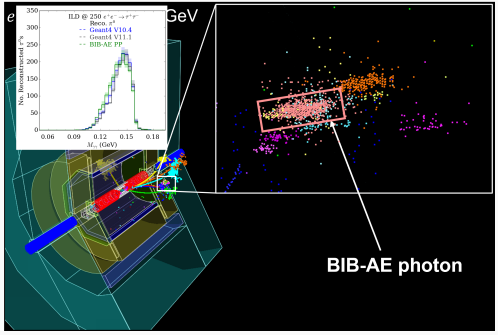
Usage:

```
>>> ga = GaudiApp()
>>> ga.setVersion('key4hep-latest')
>>> ga.setExecutable("k4run")
>>> ga.setSteeringFile('k4simdelphesalg_pythia.py')
>>> ga.setPythia8Card('p8_ee_ggqq_ecm91.cmd')
>>> ga.setExtraCLIArguments("--GenAlg.PythiaInterface.pythiaca
>>> ga.setEnergy(91.2)
>>> ga.setNumberOfEvents(50)
>>> ga.setOutputFile('output.root')
```

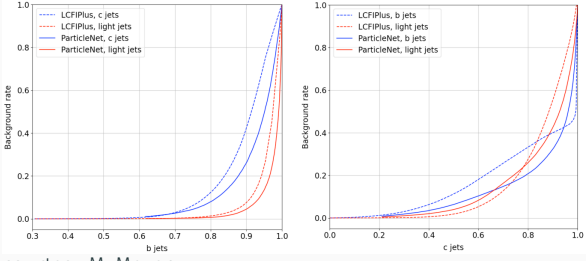
see the documentation

Using Key4hep for new developments

- DDFastShowerML - integration of generative shower models into DD4hep
  - Study reco of ML gen. showers
- See P. McKeown's PhD thesis
- More ML models integrated



courtesy P. McKeown

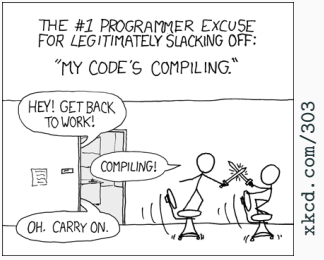


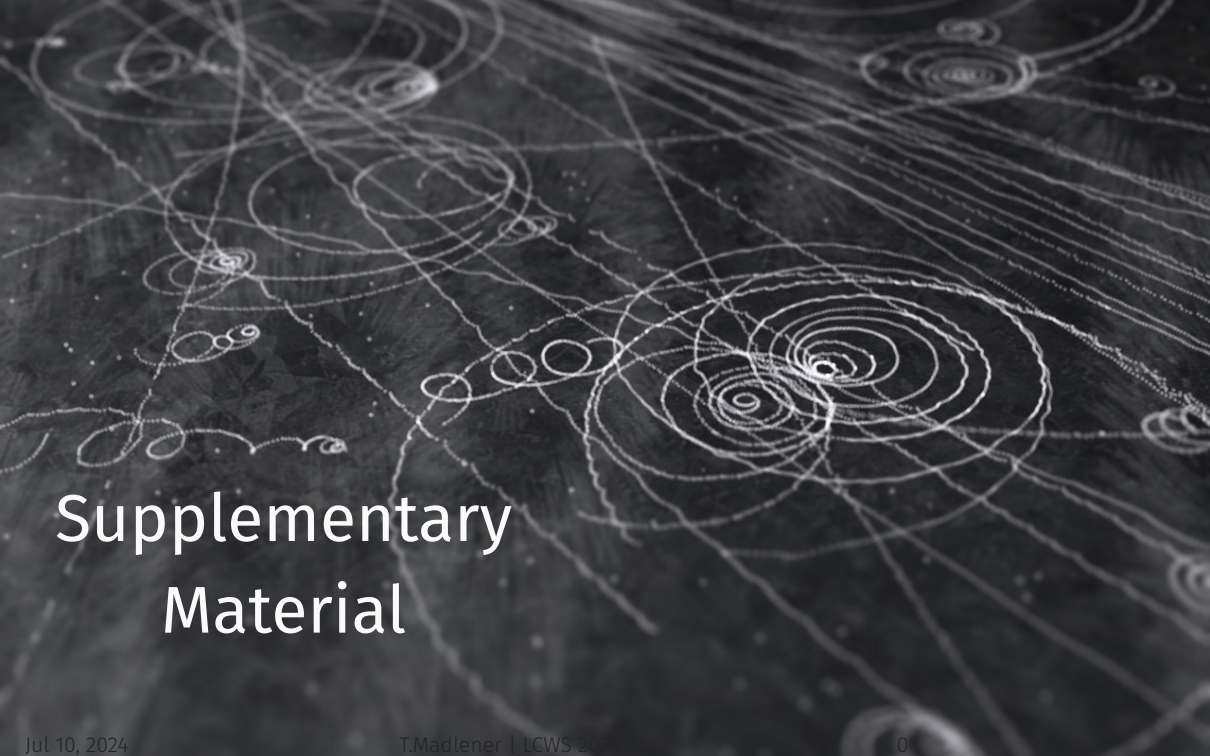
courtesy M. Meyer

- MarlinMLFlavorTagging - Using deep ML flavor taggers w/ Marlin
- Basis for similar developments in Gaudi
- Avaialable in Key4hep nightlies

Summary & Outlook

- Key4hep provides a common software stack for all future collider projects
- **Very successful in bringing together communities and focusing on common approaches**
- Existing reconstruction & analysis software from iLCSoft works unchanged
- Currently finalizing first stable versions of core components
- Migration towards “Key4hep native” ongoing for ILD
- Still lots of work ahead
  - Many exciting possibilities

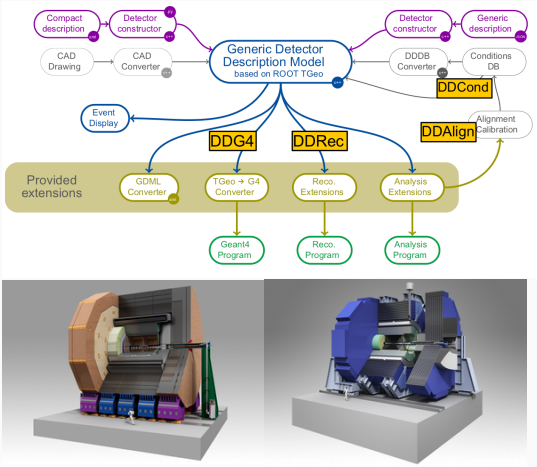



Supplementary
Material

DD4hep - Detector description

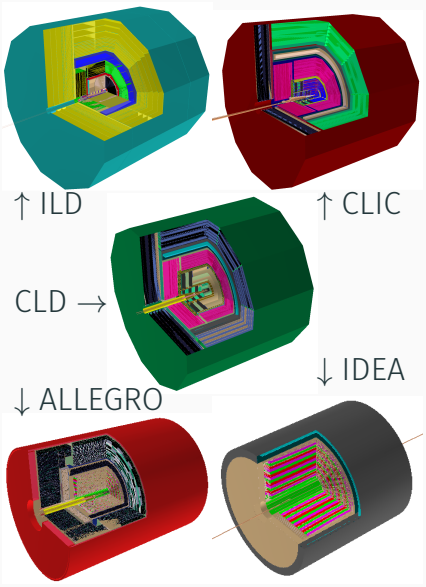
dd4hep.web.cern.ch

- Complete detector description
  - Geometry, materials, visualization, readout, alignment, calibration, ...
- From a **single source of information**
  - Simulation, reconstruction, analysis
- Comes with a powerful plug-in mechanism that allows customization
- More or less “industry standard” now
  - FCC, ILC, CLIC, EIC, LHCb, CMS, ODD, ...
- `ddsim` - standalone simulation executable

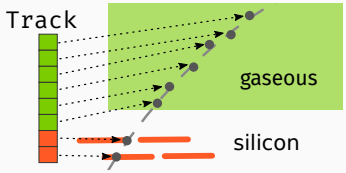


k4geo - The detector geometry repository

- Central repository for detector models
- Many existing detector models from LC studies
- Many recent developments for FCC detector concepts
- “Plug and play” approach for subdetectors
  - Use CLD inner tracker in ILD for TPC studies at FCC



Interface types and their use in EDM4hep




```yaml
interfaces:
  edm4hep::TrackerHit:
    Types: [edm4hep::TrackerHit3D, edm4hep::TrackerHitPlane]
    Members:
      - edm4hep::Vector3f position [mm] // hit position

datatypes:
  edm4hep::Track:
    OneToManyRelations:
      - edm4hep::TrackerHit trackerHits // hits of this track
```

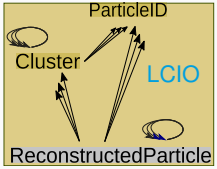
```cpp
auto track = edm4hep::Track{};
track.addHit(edm4hep::TrackerHit3D{});
track.addHit(edm4hep::TrackerHitPlane{});

const auto hits = track.getHits();
hits[0].isA<edm4hep::TrackerHit3D>(); // <-- true
hits[0].as<edm4hep::TrackerHit3D>();  // <-- "cast back"
hits[1].isA<edm4hep::TrackerHit3D>(); // <-- false
hits[1].as<edm4hep::TrackerHit3D>();  // <-- exception!
```

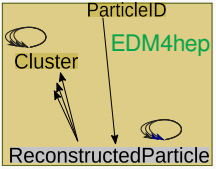
- General interface can be useful to "gloss over some details"
- Value semantics prevent inheritance based approach
  - Pointers in interfaces break consistency
  - No base class to inherit from
- Introduce *interfaces* as new category in YAML definition
  - Define desired functionality
  - **No collections!**
  - Use like normal *datatypes*
  - "Casting back" is possible

ParticleID handling EDM4hep vs LCIO

- Remove `ParticleID` relation from `Cluster`
  - Found no usage in ILD / CLIC reconstruction
- Make `ParticleID` have a one-to-one relation to `ReconstructedParticle`
  - Also remove `particleIDUsed`
- `ParticleID` has been (ab)used in LCIO as *transient parameter (values) store*
  - Will require change of pattern for EDM4hep
- Simple use cases become simpler with EDM4hep
- Tooling keeps the rest at the same level
- Some usability improvements wrt LCIO
  - keyhep/EDM4hep#298

key4hep/EDM4hep#268





ParticleID related utilities

- `edm4hep::utils::PIDHandler` similar to `UTIL::PIDHandler`
  - Get related `ParticleID`s from a `ReconstructedParticle`
  - Retrieve some PID metadata
  - Slightly more modern interface for EDM4hep
- Handling of necessary metadata very different
  - LCIO: *collection parameters* - tight coupling
  - EDM4hep: *file level metadata* - looser coupling
  - Gory details here and here
- See the documentation for more usage examples
- **Feedback very much appreciated!**

ParticleID handling comparison

Getting the dE/dx distance wrt an electron for all particles

```cpp
using namespace EVENT;
using namespace UTIL;

auto recos = event->getCollection("PandoraPFOs");
auto pidHandler = PIDHandler(recos);

const auto dEdxId = pidHandler.getAlgorithmID(_dEdxname);
const auto dEdx_e_Id = pidHandler.getAlgorithmID(dEdxId,
                                                 "e_dEdx_dist");

for (int i = 0; i < recos->getNumberOfElements(); ++i) {
  auto p = static_cast<ReconstructedParticle*>(
             recos->getElementAt(i));

  if (p->getCharge() == 0.0) {
    continue; // only charged particles have tracks
  }

  const auto& dEdxParams = pidHandler.getParticleID(p, dEdxId);
  const auto dEdx_e_dist = dEdxParams[dEdx_e_Id];

  // do something with the particle and the dEdx distance
}
```

LCIO

```cpp
using namespace edm4hep;
using namespace edm4hep::utils;

const auto dEdx = event.get<ParticleIDCollection>("dEdx");


const auto dEdxMeta = PIDHandler::getAlgoInfo(metadata, "dEdx");
const auto dEdx_e_Id = getParamIndex(dEdxMeta, "e_dEdx_dist");


for (const auto pid : dEdx) {
  const auto p = pid.getParticle();









  const auto dEdxParams = dEdx.getParameters();
  const auto dEdx_e_dist = dEdxParams[dEdx_e_Id];

  // do something with the particle and the dEdx distance
}
```

EDM4hep