WP7 Software

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CERN EP R&D Day

2024-05-22

Introduction

Trends in HEP Software and Computing

Software is ubiquitous in HEP

- Event generation, simulation, trigger, reconstruction, analysis

Challenges for future experiments

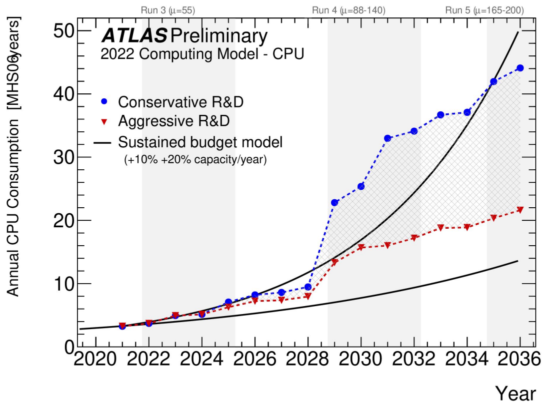
- Event rates
- Event complexity
- Precision physics

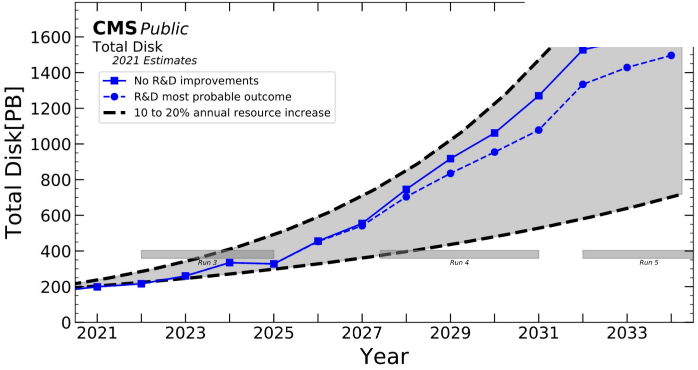
Challenges for Future Collider Studies

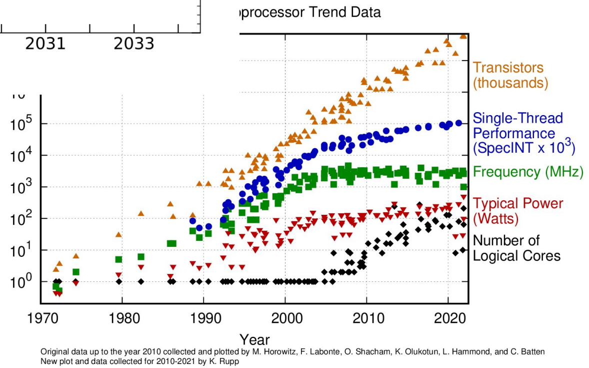
- Agile and sophisticated software
- Speed and accuracy of algorithms
- High statistics

Plus… difficult trends in

- Computing hardware
- Storage technology
- Energy costs, a.k.a., Green Computing

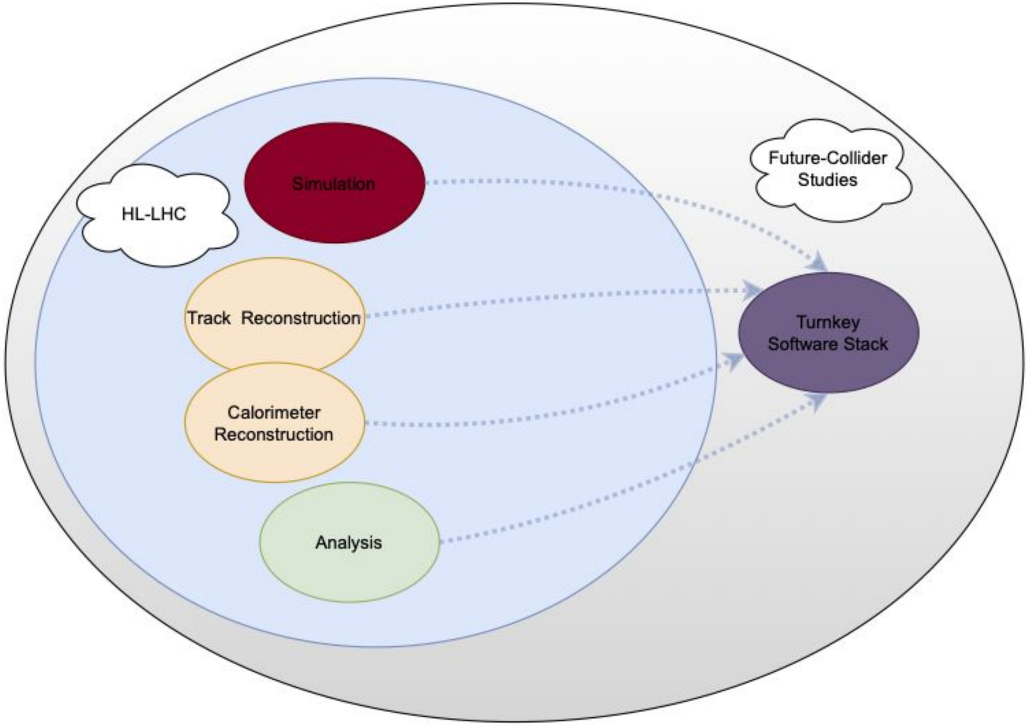






EP R&D Phase 1

- Address key components of future needs (HL-LHC and future experiments)
  - Faster Simulation
  - Tracking and Calorimeter Reconstruction
  - Faster Analysis
- Supporting Future Collider Studies with ‘best of breed’ components
  - Turnkey Software Stack - this is a testbed for other developments

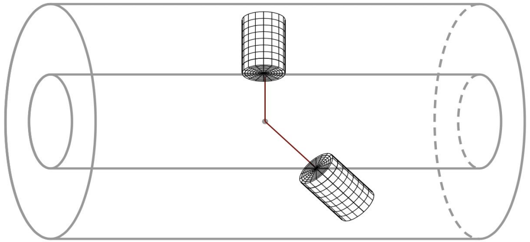


Towards Phase 2

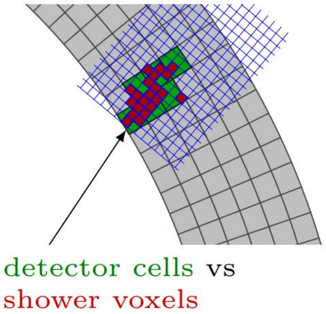
- Timescales
    - Software programme that still applies to the HL-LHC and the continual software evolution that will occur
        - Future upgrades for LHCb and ALICE (Run 5) enter more into scope
    - Continue to support more and more refined future detector studies
- Key motivations for software remain
    - We continue the primary thrust of many of the tasks
    - Some evolve significantly, e.g., in Turnkey moving to more specific framework R&D
    - Core Libraries is a new line of work
    - Common themes develop and are an important unifying feature of the R&D proposal
        - Open Data Detector
            - Neutral testbed for algorithm development and open datasets
        - GPU Support and expertise
            - Building knowledge across tasks in how to use and support GPU code
            - HEP geometry, field maps, core mathematical operations, etc.
        - Hardware diversity - shared resources between tasks
- Partners
    - We work in collaboration with several non-CERN institutes and initatives (DESY, IJCLab, IHEP, IBM, openlab), also, in particular through AIDAinnova

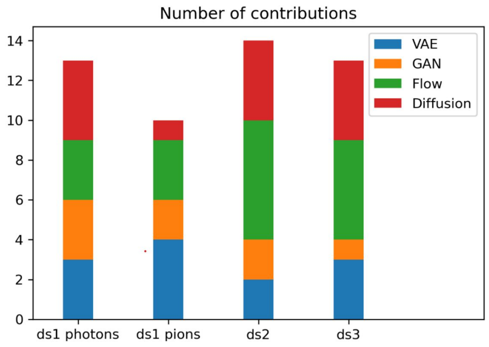
Faster Simulation with ML

EP R&D Phase-1 outcomes

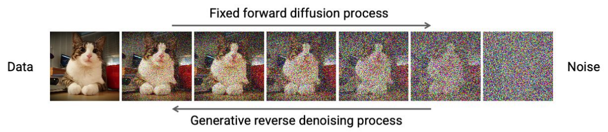


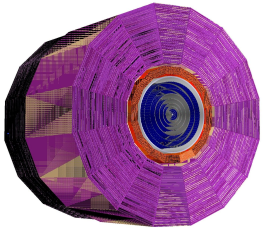
- Par04 - Geant4 example for ML-based Fast Simulation
  - Detector-readout independent showers (released on Zenodo)
  - Training and conversion (ONNX, LWTNN, LibTorch) of ML model
  - Inference in Geant4 (putting the generated hits back)
  - Released in Geant4 11.2 - including GPU support
  - Adoption of some of these tools for Gaussino, LHCb
- MetaHEP - a model able to adapt quickly to new detectors
- Easy to use pipeline in Kubeflow with automatic hyperparameter optimization in Katib
- Co-organization of CaloChallenge, ML competition for encouraging development and better understanding of FastSim.
  - Datasets of varying complexity (including Par04)
  - Various metrics for benchmarking and objective comparison



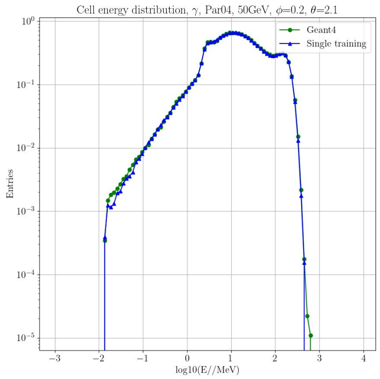


EP R&D Phase-1 outcomes

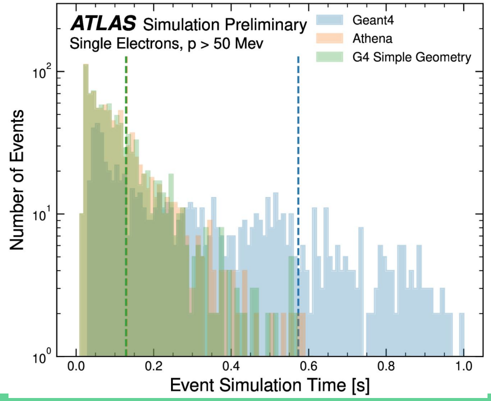




- Contributions to developing Open Data Detector (ODD)
  - Realistic detector geometry for algorithmic research and development purposes
  - Updates presented at ML4Jets2023
- Development of CaloDiT, a transformer-based diffusion model
- Proof of concept on extending the models to more realistic geometries like FCCee (ALLEGRO, CLD) and ODD
- Investigated realistic limits on speedup using FastSim, O(10^3)
- Contributions to developing experiment-independent fast calorimeter simulation library from ATLAS FastCaloSim (AF3)
  - Replaced ATLAS particle transport with Geant4 transport
  - Decoupled most of FastCaloSim code from Athena software



CaloDiT on Par04



For EP R&D Phase-2 - Ongoing and future work

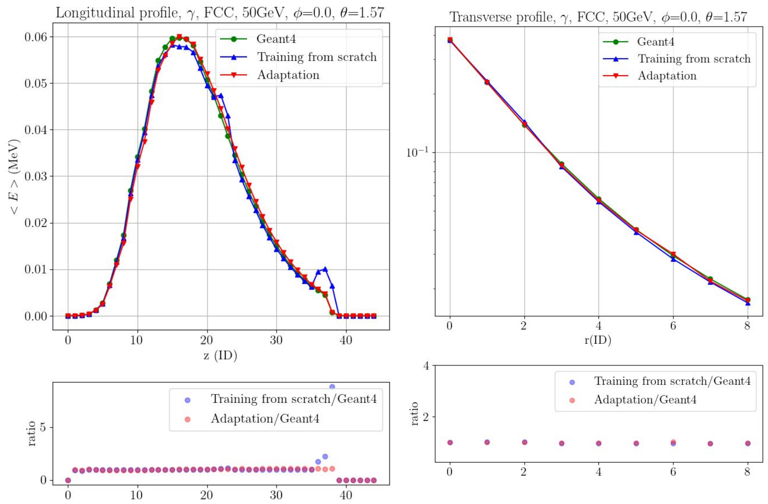
- Development of a Foundation model for FastSim (CaloDiT)
  - Train once on multiple geometries and quickly adapt to new ones
  - In collaboration with IBM and Openlab

Future work

- Scaling CaloDiT in terms of dataset and model size
- Optimization of CaloDiT
- Inference in DD4hep for studying effects of reconstruction
- Testing models in ATLAS software
- Ongoing support for LHCb fast sim development

[EP R&D Day Poster “Towards detector agnostic Fast Simulation”]

Pretraining on Par04 & ODD, and adaptation to FCCeeALLEGRO



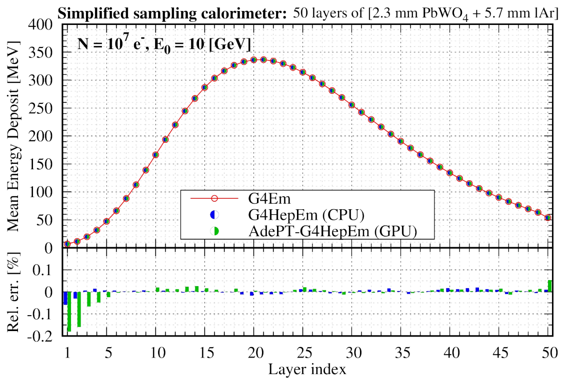
250 epochs of training from scratch (blue) are required match 20 epochs of adaptation (red)

~12x less training time

Faster Simulation on GPUs

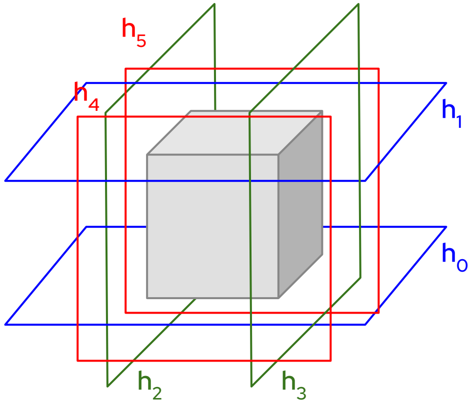
AdePT status

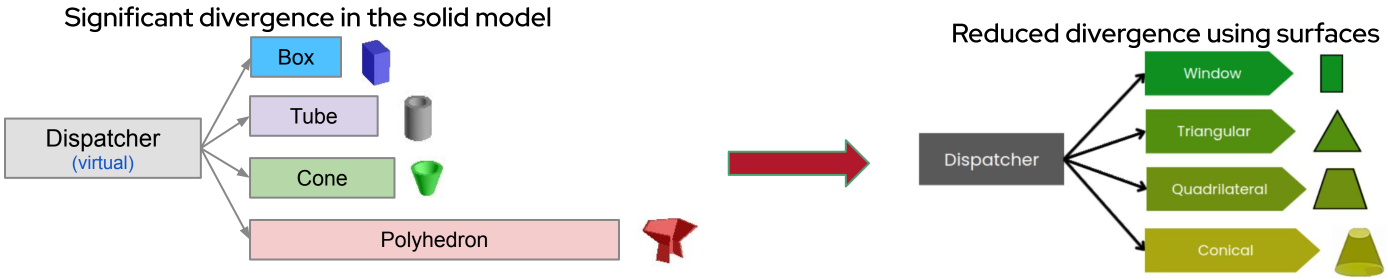
- Achieved the initial goals of the R&D
  - Understand usability of GPUs for general particle transport simulation, seeking for potential speed up and/or usage of available GPU resource for the HEP simulation
    - Prototype e+, e− and γ EM shower simulation on GPU, evolve to realistic use-cases
      - Geometry: VecGeom library, Physics: G4HepEm library
- Transport for EM particles working on GPUs for LHC-complexity geometries
  - Excellent physics agreement within statistical fluctuation
  - Reproducibility of the simulation achieved
- Full integration with Geant4 applications
  - Possible to plug AdePT into existing Geant4 applications with minimal extra code
    - reusing existing sensitive detector implementations
- Main bottleneck: geometry – being addressed now (see following slides)



Bounded surface modeling for improving GPU performance

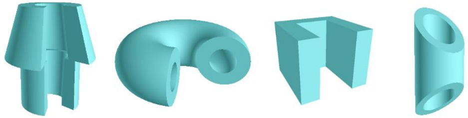
- Portable GPU-friendly header library
  - Algorithmic part independent on the backend, compilable with any native/portability compiler
  - Headers templated on the precision type to allow for a single-precision mode
- Code simplification and GPU performance
  - No virtual calls, no recursions, more work-balanced
  - Better device occupancy and kernel coherence
  - Reducing divergence and register usage on the GPU





Status and plans

Surface model supports **all solids** required by the experiments

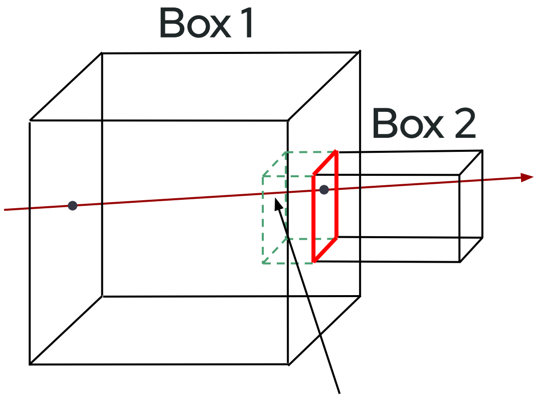


Current priorities:

- Debugging complex geometries (CMS, LHCb): **Overlaps** require relocations
- Implementing **Bounding Volume Hierarchy** accelerating structure

Next:

- Performance measurements, testing calorimeters (ATLAS EMEC, CMS HGCAL, LHCb ECAL)
- Lightweight portability layer (instead of pure CUDA)



Missing the overlapping entering surface leads to missing Box 2 entirely

Track Reconstruction

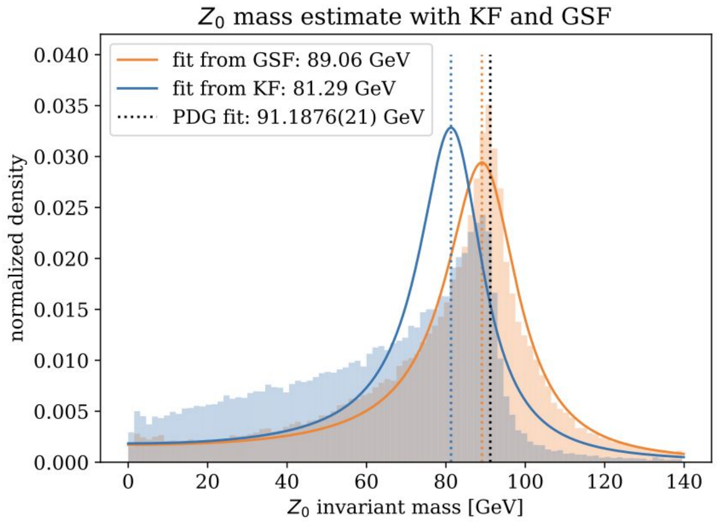
EP R&D Phase 1 - Modern track reconstruction

Established a strong, feature-rich CPU baseline of track reconstruction
[P. Gessinger-Befurt, M. Kiehn, A. Salzburger et al, CSBS2022]

- detector agnostic yet customizable
  clients: ATLAS, FASER, sPHENIX, ePIC, ...
- high performant
  physics performance, computing performance
- extendable

EP R&D initiative was extremely helpful to develop and define common interfaces

- Geometry (DD4hep, GeoModel)
- EDM (EDM4hep, PODIO)



Gaussian Sum Filter in ACTS

EP R&D Phase 1 - Outcome and further R&D

Commonly* developed OpenDataDetector

[E. Brondolin, P. Gessinger-Befurt, A. Salzburger, D. Salamani, A. Zaborowska, et al, CHEP2023]

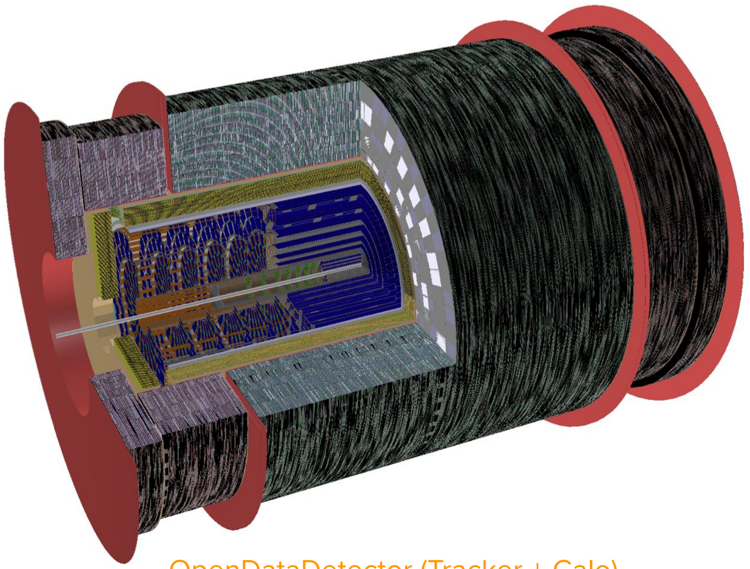
- to develop and showcase algorithms & performance
  [P. Gessinger-Befurt, A. Salzburger, et al, CTD2023]

EDM frontend/backend separation

- PODIO/EDM4hep demonstrators
  [P. Gessinger-Befurt, CHEP2023]

Geometry (detray) and Simulation support for GPU R&D line traccc

- Exchange with AdePT on GPU geometry



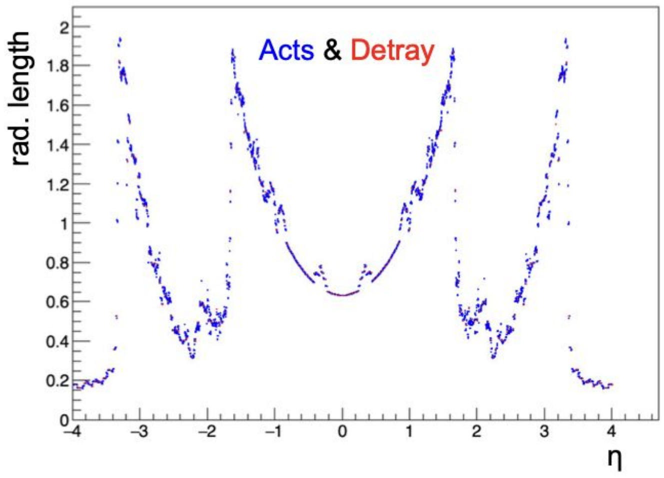
OpenDataDetector (Tracker + Calo) defined in DD4hep, used in ACTS/DDSim

*with EP R&D members from the fast simulation activity

Towards Phase 2

Shift focus to GPU R&D & **improve integration into Key4hep for FCCee**

- New geometry model allows easier binding to DD4hep, EDM4hep converters in place
- Re-establish full track reconstruction chain with time information: CPU/GPU code
- Enhance detray geometry for Calorimeter
  Simplified geometry building from DD4hep
- Develop full parameter transport through calorimeter with dense material
  Input for combined (time-aware) particle flow algorithms
- Combine with Calorimeter Reconstruction task to support modern particle flow algorithms

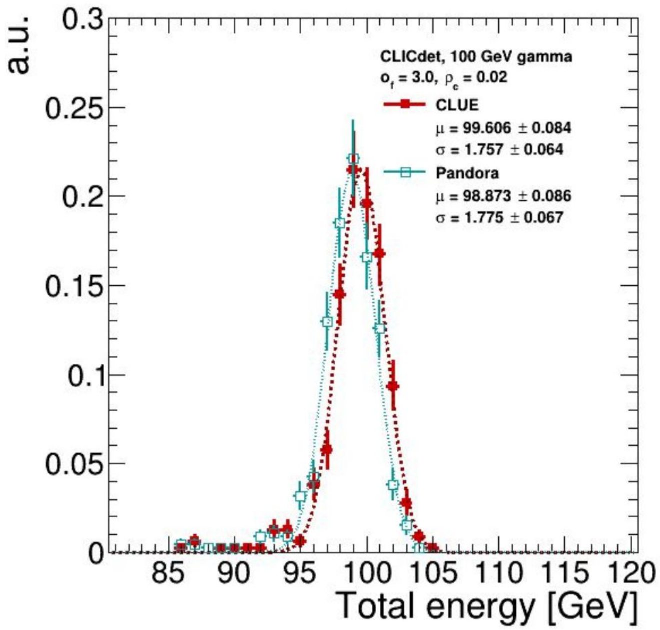


Achieved quasi-identical material (shown) and magnetic field accuracy on CPU/GPU

Calorimeter Reconstruction

k4CLUE: CLUE integration in Key4hep

- CLUE: fast density-based **clustering algorithm** already in use in HGCAL reconstruction
  - uses **energy density** to establish seeds, outliers, and followers in 2D planes
  - **GPU**-friendly
- Key4hep integration:
  - adapted to the common event data model, **EDM4hep**
  - adapted to run on **full detector**
  - supports **different** type of **calorimeter** layouts
  - github CI and EDM4hep **Validation**

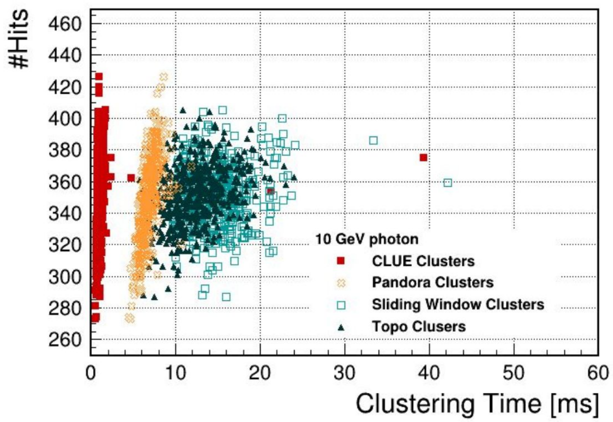


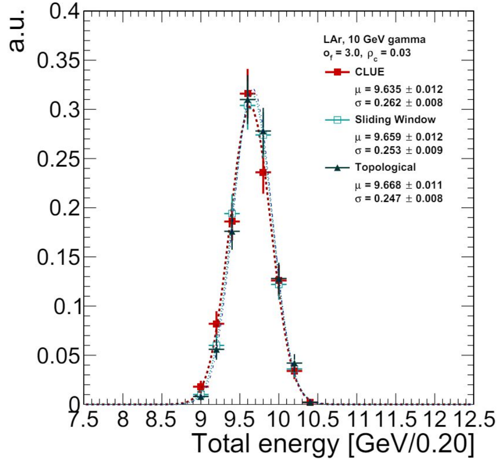
Brondolin E., Pantaleo F., Rovere M., [The k4Clue package: Empowering Future Collider Experiments with the CLUE Algorithm]

k4CLUE: performance results

Analysis on three different future calorimeters for single gamma events:

- similar performance with respect to other baseline algorithms
- **good performance** in presence of noise
- clear **advantage** in terms of **timing** performance
  - not dependent on the number of input hits
  - **only CPU version used, GPU version would be even faster**





Brondolin E., Pantaleo F., Rovere M., *k4Clue: the CLUE Algorithm for Future Collider Experiments*, CTD2023

Towards Phase 2

- Integrating the k4Clue developments in the kalos/CLUE generic library with GPU support
- Testing and porting to GPU CLUE3D (clustering across full calorimeter)

Explore new solution for the pattern recognition with timing:

- Explore the time information available in the FCC detectors
- Integrate time information in pattern recognition algorithms in calorimeters reconstruction in CMS and FCC
  - plan to adapt HGCAL algorithmic techniques in the context of detectors foreseen for future collider experiments
- In the long run, combination with tracker info coming from 6D Kalman filter to perform a time-aware global event description

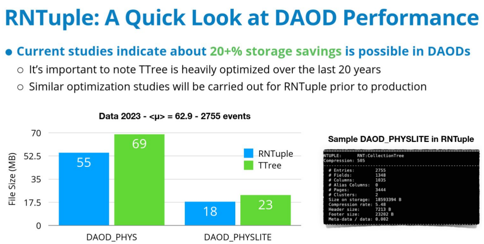
Faster Analysis

Faster analysis: I/O and programming model

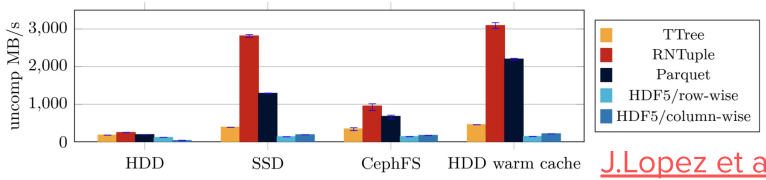
Phase I: Two-fold strategy to enable next-generation HEP analysis

- Rewrite the HEP I/O layer
  - **RNTuple**: the future experiment data format
  - **2-5x** throughput **speedup** on fast storage devices w.r.t. **TTree**
  - Best-suited for HEP requirements compared to industry-standard tools
  - File-based **and** object storage (i.e. HPC and cloud)
  - **20% storage savings** for **ATLAS** production!

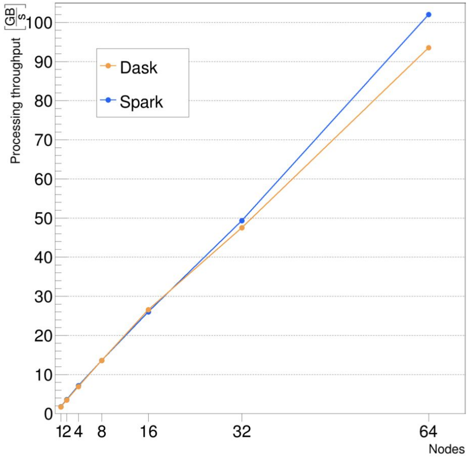
- Enable scaling an analysis to thousands of cores
  - Distributed RDataFrame **runs everywhere**
  - One API that unifies all HEP analyses, from a laptop to a Grid site
  - Performance tested up to thousands of cores



S. Mete et al.



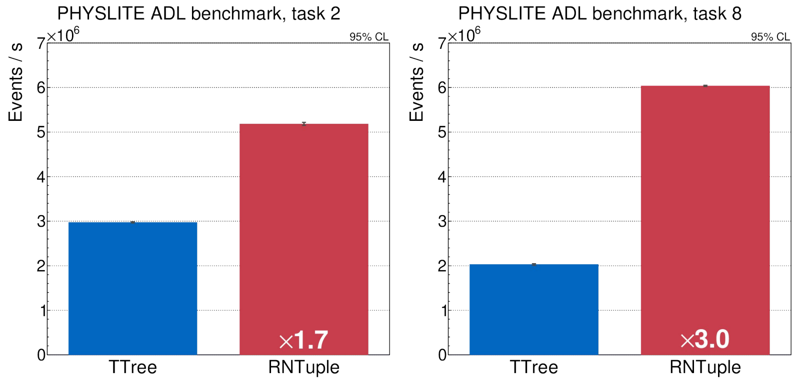
J.Lopez et al.



V. E. Padulano et al.

Since last year: smooth I/O and analysis integration

- RNTuple gives more performance and smaller dataset sizes
  - At no cost for the final user
- 1:1 compatibility with RDataFrame analysis
  - The tool can automatically detect TTree/RNTuple datasets
- Natively parallel: multithreaded or distributed analysis
  - RDataFrame+RNTuple+SWAN (ACAT'24)
  - Running a standard community benchmark with multi TB dataset (AGC)



1 top-level field read,
no cuts/calculations applied

12 top-level fields read,
basic cuts/calculations applied

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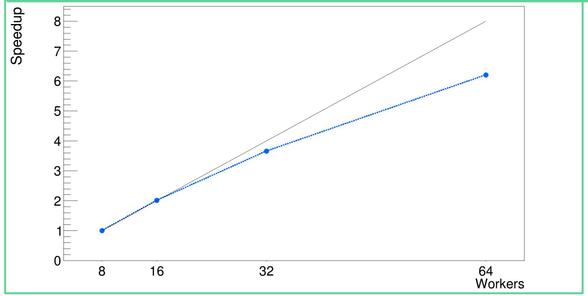
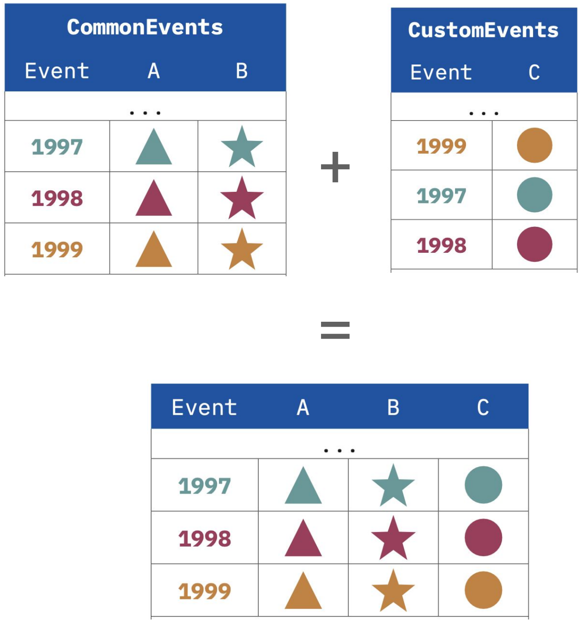


Looking at Phase 2

- Challenge: complex event matching of RNTuple datasets
  - Gather **desiderata** from **real** community use **cases**
  - Extend TTree compositions (chains, friends)
  - 1:1 or **1:N** relationships, **unaligned** events in the datasets
  - Provide **API** for **higher-level** tools
  - Ensure similar performance for most use cases
  - Vertical concatenations require clear definition of assumptions
  - Potential for significant storage savings by not duplicating columns into new files
- Validation at realistic scales
  - Also in collaboration with the community (CERN IT, experiment frameworks)
  - Test and benchmark on various HPC sites
- Future-proof the data format
  - Schema evolution, backwards and forwards compatibility features

F. de Geus: EP R&D Day Poster



HEP Core Libraries (New Task)

Core Libraries

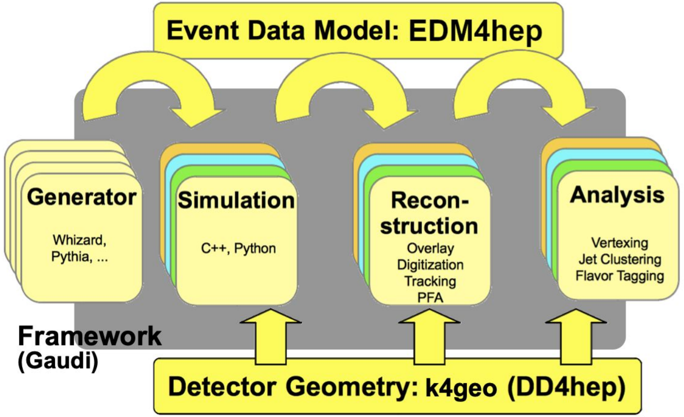
- Future experiments' will have huge and complex data sets
  - This requires a new platform of reengineered HEP foundation libraries and interfaces
    - Take advantage of the increasingly wide variety of modern computing devices, ergonomically
  - Not adapting to these trends is a considerable risk, which we mitigate with this work
- **Histogramming on GPUs**
  - Develop a new accelerator friendly histogram package for HEP, offering modern interfaces
  - Start by investigating ways to implement efficient data accumulation on accelerators and ensure that this functionality is interoperable with existing ROOT histogramming
  - The development of this new library will leverage the experience of ROOT's and experiments' existing implementations

Core Libraries

- **Sustainable C++-Python interoperability**
  - Current adoption trends suggest that in the 2030s most analyses will be written in Python
  - To keep usage of HEP's highly efficient C++ libraries high, effort will be invested in HEP's critical and unique Python binding, PyROOT
  - PyROOT has existed for many years within the ROOT package, it iss very powerful since it is based on the Cling C++ interpreter (in the LLVM compiler suite)
    - However, needs to become more sustainable
  - Start by investigating new kinds of bindings to complement or replace the existing ones which are created dynamically
  - Assess the feasibility of upstreaming parts of cling/PyROOT to LLVM, thereby sharing their support cost with the community
  - Identify an ergonomic way to provide the new histograms developments in Python

Turnkey Software

Key4hep: Turnkey Software Stack



- Developed the complete turnkey software stack from simulation to analysis
  - Integrated FCC and CLIC frameworks into common software stack
  - Crucial for FCC feasibility study detector studies
- Successfully build up an international community with participants from CEPC, CLIC, EIC, FCC, ILC, Muon Collider from CERN, DESY, IHEP, INFN, et al.
  - Endorsed for ECFA Higgs/EWK/Top factories studies
- Key4hep has become an established platform with increased adoption from developers in the contributing projects

EP R&D Day Poster: "Key4hep: a Turnkey Software Framework for Future Accelerator Experiments"

EP R&D in Key4hep

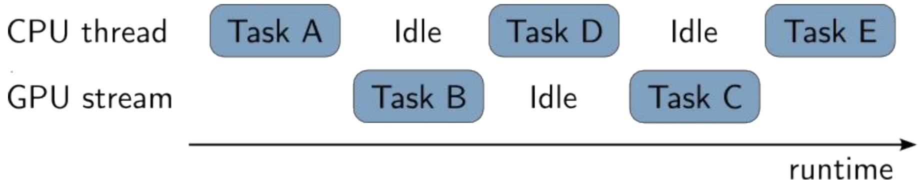
- **Crucial** contributions from EP R&D
  - Key4hep stack (nightly builds and stable releases) with over 500 packages on cvmfs
  - Integration with Gaudi for running reconstruction algorithms
    - Ongoing developments: tracking with ACTS, Pandora particle flow, overlay and more
  - In-memory dynamic conversion between LCIO (used by the ILC community) and EDM4hep, allowing algorithms that use either EDM4hep or LCIO to work together
  - Full reconstruction pipeline used as validation for detector design and development
  - Developments in podio and EDM4hep, like RNTuple support
  - Continuous validation system, improvements to software development

- Outlook for Key4hep
  - Consolidate and finish a stable version of EDM4hep
  - Participate in and benefit from the FCC studies
    - Increase in activity already happening
  - Needs continued input and sustained effort to continue to support the production mode

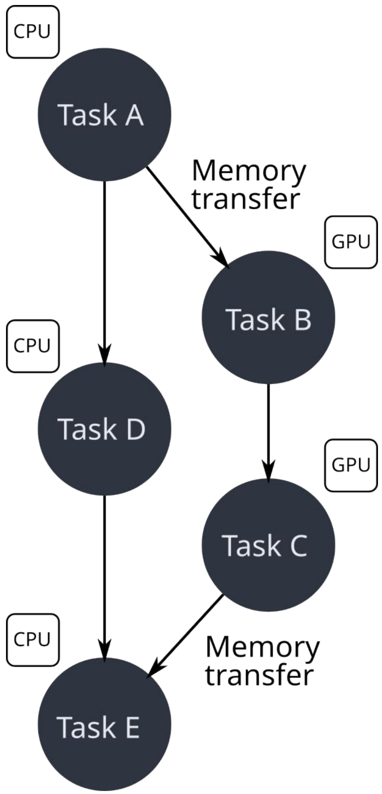
Heterogeneous Frameworks

Scheduling with heterogeneous resources

- Heterogeneous resources becoming more and more available and increasingly important for HPC
- Concurrent schedulers adopted by the experiments a decade ago
  - Main focus on multi-process and thread-parallel execution
  - Successful ad-hoc solutions for multi-node setups, non-blocking tasks and computation offloading



- New 3rd party libraries, frameworks and computing models for heterogeneous scheduling available
- Prototype new heterogeneous schedulers for future experiments
  - While learning and incorporating prior experience of CMSSW and Athena



Heterogeneous scheduling status and plans

Phase I - now

- **Done**: Extracted information about workloads used by the experiments:
  - Data flow and control flow graphs
  - Algorithm timings and now as well data object memory footprints
    Presented at Gaudi Developer Meeting
- **Ongoing**: Prototype single-node scheduler with asynchronous offloading
  - Create demonstrators running mockup workloads
  - Started to evaluate the state-of-the-art task-graph heterogeneous scheduling libraries and different multi-tasking styles (cooperative scheduling)
- **Ongoing**: Investigate scheduling in new programming languages:
  - Prepare demonstrator in Julia using Dagger.jl framework, repository
  - Working with an Ukrainian Remote Student and soon with an additional Summer Student

Phase II - longer-term

- Distributed scheduling with multiple nodes and architectures
- Study energy-efficient scheduling with heterogeneous nodes
- Implementation strategies for next generation frameworks

Summary and Conclusions

EP Software R&D Summary

- Phase 1 of the Software Work Package of EP R&D achieved a great deal
  - Working high-performance software stack supporting FCC studies and used by many future experiment studies
  - R&D into advanced ML simulation techniques for calorimeters
  - State of the art reconstruction techniques for trackers and calorimeters
  - Development of world class performant file format for HEP, with ergonomic analysis interfaces
- We look forward to continuing these strong lines of development and adding new ones
  - Improved frameworks support for heterogeneous environments
  - Particle tracking on GPUs
  - Core library support for GPUs
  - Full incorporation of timing into reconstruction, with “full-event” understanding
- R&D with strong links to current and future experiments
  - Aim at early adoption into production as soon as possible

Backup

Adaptation using CaloDiT

FCCeeALLEGRO

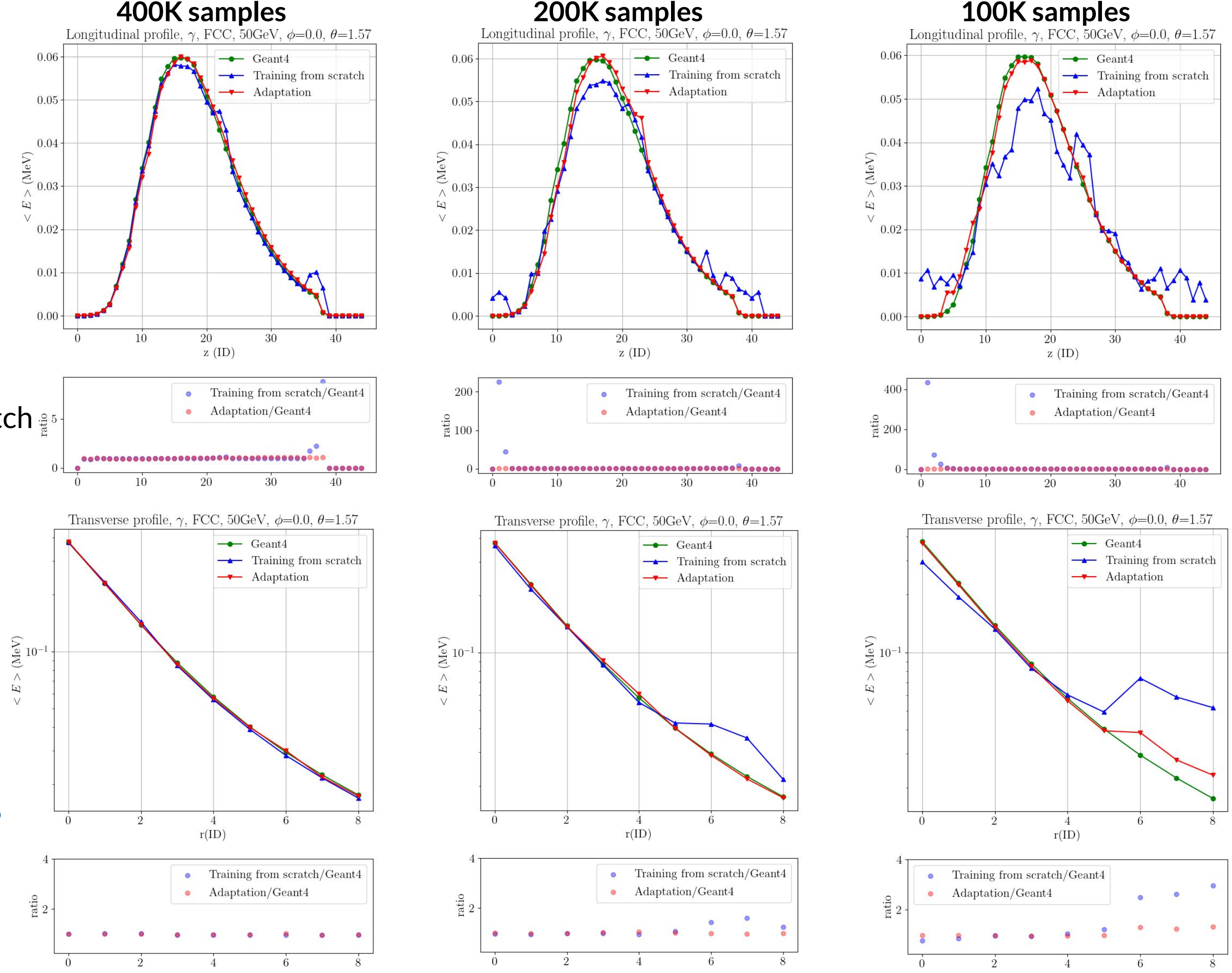
250 epochs for training from scratch
20 epochs for adaptation

At 200K samples

~25x less training time

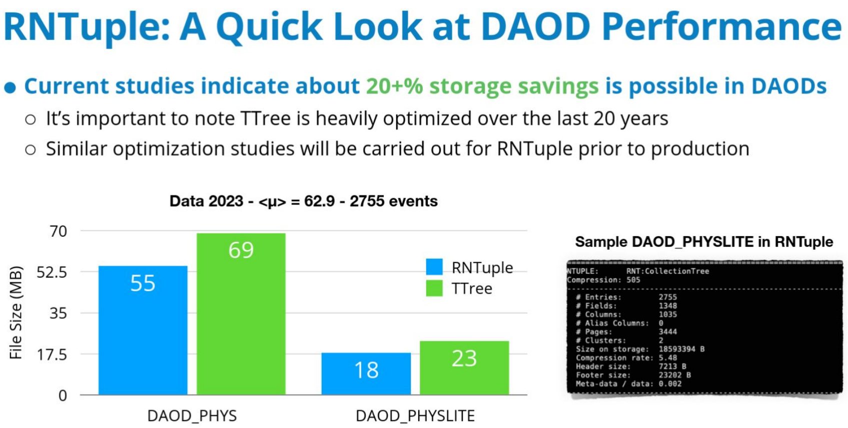
<50% of the data

Preliminary results



RNTuple: the path to production

- RNTuple workshop 2023 (indico)
  - Participation of LHC core computing devs, CERN IT, HEP-CCE
- Work towards the release of a stable binary format
  - Allows stakeholders to battle test future data pipelines
  - RNTuple API review by external experts (HEP-CCE)
- Integrating RNTuple in experiment production
  - All ATLAS data products available, most of CMS
  - +20% storage saving in ATLAS DAODs

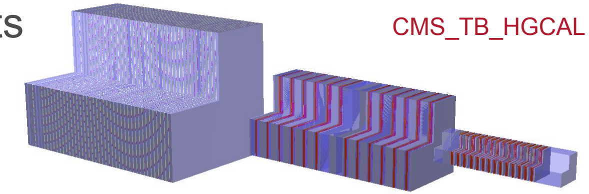


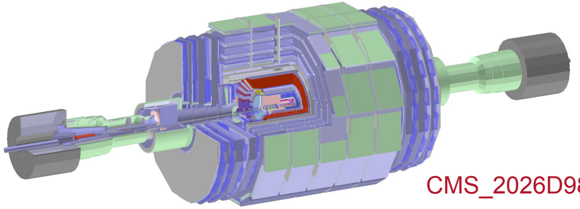
ACAT `24, S. Mete

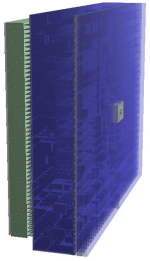
VecGeom surface model targeting GPUs

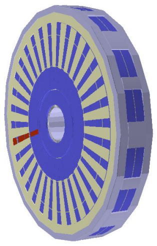
Surface model now supports **all solids** used by the experiments
- conversion time and memory footprint under control

	# touchables [million]	conversion time [s]	memory [MB]
cms_2018	2.1	3.0	102
cms_TB_HGCAL	0.06	0.5	28.4
cms_2026D98	13.1	18.0	278
LHCb_Upgrade	18.5	19.5	106
LHCb_ECal_HCal	18.4	0.3	4.4
ATLAS_EMEC	0.08	0.9	62.6


CMS_TB_HGCAL


CMS_2026D98


LHCb_ECal_HCal


ATLAS_EMEC