热烈欢迎各位参加

粒子物理实验计算软件与技术研讨会

2023年6月9-12日

相关系列会议

- 2013年7月： 粒子物理实验计算软件与技术研讨会（威海）
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- 2017年6月： 高能物理计算和软件会议（成都）
- 2019年5月： 高能物理计算和软件会议（南京）
- 2019年7月： BESIII 软件与计算研讨会（青岛）
- 2022年11月：BESIII软件与计算研讨会（北京）

Overview of
Software and Computing of HEP Experiments

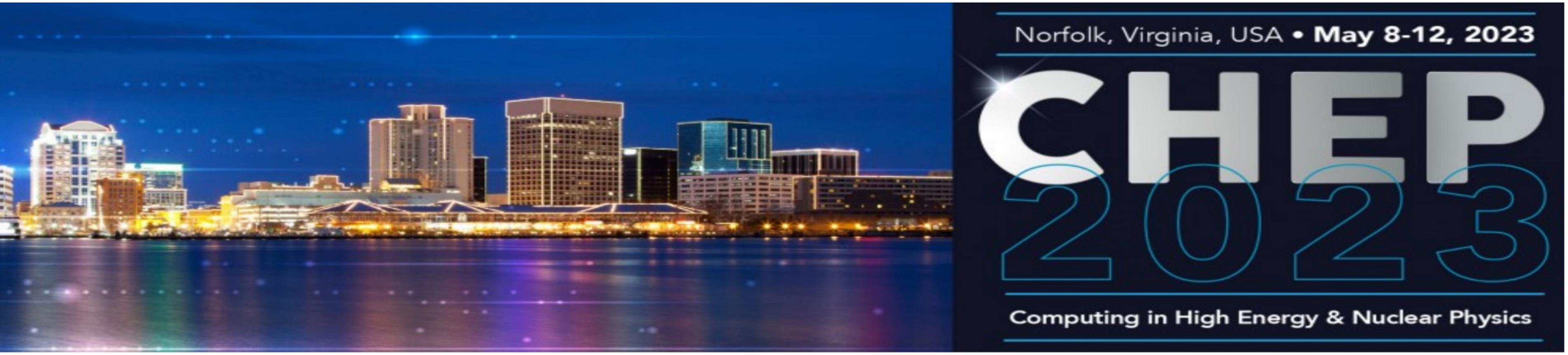
--- based on CHEP2023 Highlights

Xiaocong Ai, Wenxing Fang, Xingtao Huang, Teng Li, Weidong Li,

Tao Lin, Jiaheng Zou

June 9-12, 2023

Workshop of Computing Software and Technologies in Particle Physics Experiments
(2023, Qingdao)



- Track 1: Data and Metadata Organization, Management and Access
- Track 2: Online Computing
- Track 3: Offline computing
- Track 4: Distributed Computing
- Track 5: Sustainable and Collaborative Software Engineering
- Track 6: Physics Analysis Tools
- Track 7: Facilities and Virtualization
- Track 8: Collaboration, Reinterpretation, Outreach and Education
- Track 9: Artificial Intelligence and Machine Learning
- Track X: Exascale Science, Heterogeneous Computing and Accelerators, and Quantum Computing

CHEP2023: 高能所、山大、国科大、中山大学等单位28个报告（17个oral,11个poster）
CHEP2019: 高能所、山大、国科大、清华、西交大等单位22报告 (10个oral,12个poster）

Computational Frontier

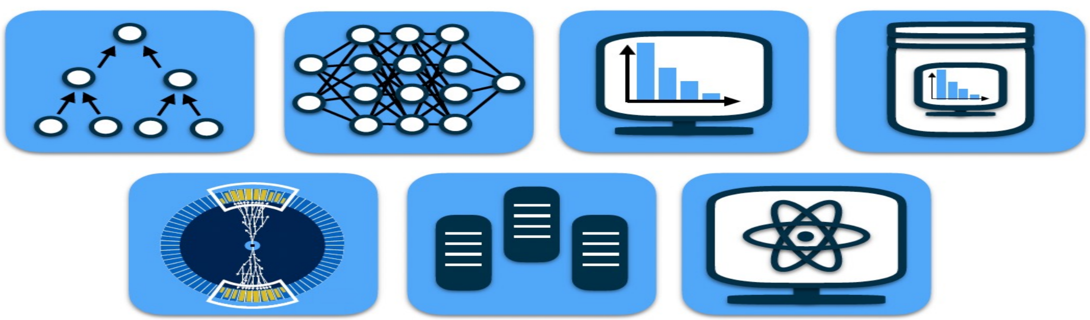
- without computing/methodological innovation, we will not be able to take full advantage of pristine data collected by state-of-the-art instruments.
- seeking solutions for specific software and computing challenges
- recognize the transformative impact of newly established (Machine Learning) and emerging (Quantum Computing) technologies

arXiv:2210.05822v3 [hep-ex] 8 Nov 2022

The Future of High Energy Physics Software and Computing

Report of the 2021 US Community Study on the Future of Particle Physics

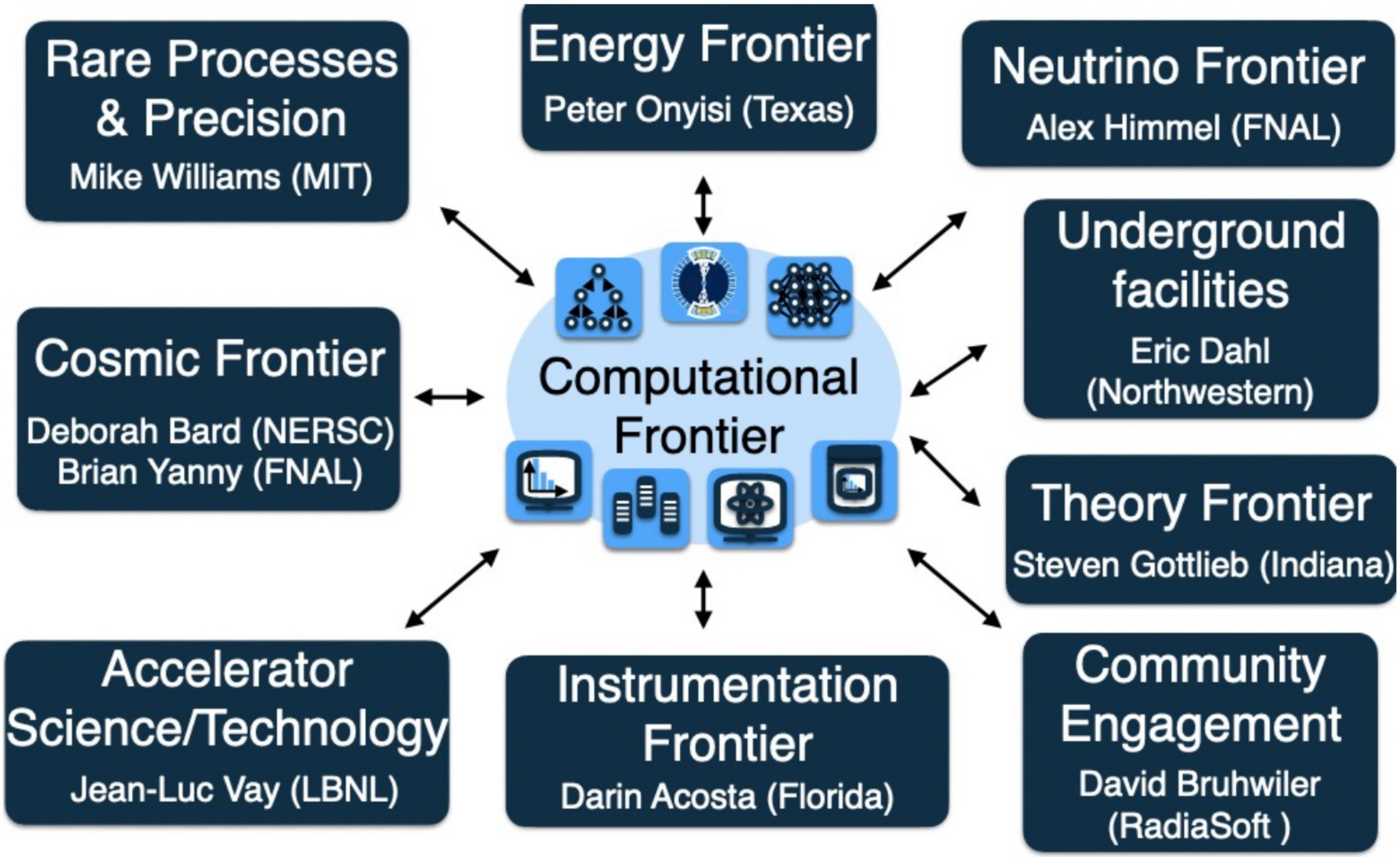
organized by the APS Division of Particles and Fields



v2.1; updated: November 9, 2022

Conveners: V. Daniel Elvira*, Steven Gottlieb, Oliver Gutsche†, and Benjamin Nachman

Computational Frontier



Computational Frontier

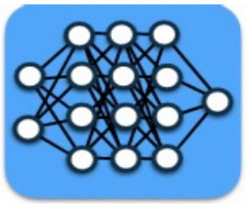
- Topical Groups

CompF01
Experimental Algorithm Parallelization

Giuseppe Cerati (FNAL), Katrin Heitmann (ANL), Walter Hopkins (ANL)

CompF02
Theory Calculations & Simulation

Peter Boyle (BNL), Kevin Pedro (FNAL), Ji Qiang (LBNL)



CompF03
Machine Learning

Phiala Shanahan (MIT), Kazu Terao (SLAC), Daniel Whiteson (Irvine)

CompF04
Storage and Processing Resource Access
(Facility and Infrastructure R&D)

Wahid Bhimji (NERSC), Meifeng Lin (BNL), Frank Würthwein (UCSD)

CompF05
End User Analysis

Gavin Davis (U. Mississippi), Peter Onyisi (U. Texas at Austin), Amy Roberts (UC Denver)

CompF06
Quantum Computing

Travis Humble (ORNL), Gabriel Perdue (FNAL), Martin Savage (U. Washington)

CompF07
Reinterpretation & Long-term Preservation of Data and Code

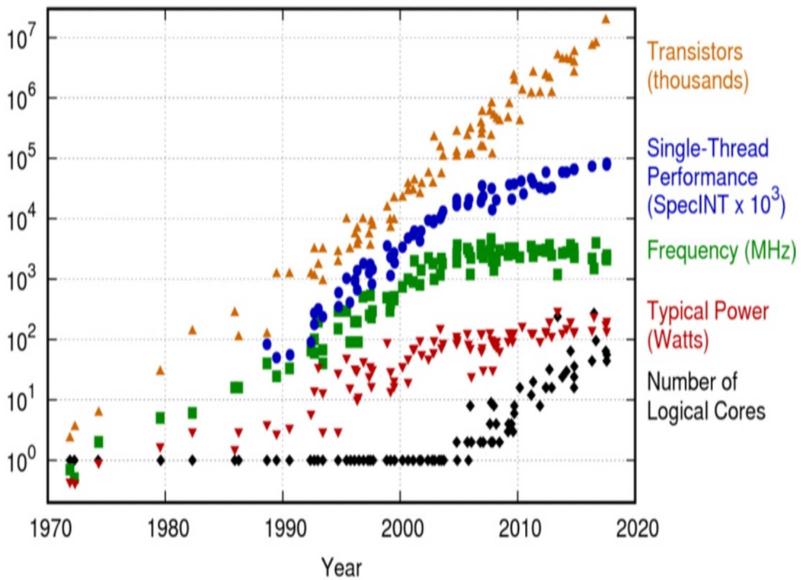
Stephen Bailey (LBNL), Kyle Cranmer (NYU), Matias Carrasco Kind (Illinois/NCSA)

Hardware evolution: a brave new world in computing

A paradigm change in computing architecture

- **Dennard Scaling (DS):** power used by silicon device/volume independent on the number of transistors
- **Moore's Law:** transistor density doubles every two years
- **Clock speed (CS):** increased 1,000 times in 1970-2000

Computer speed doubled every 2 years while cost halved



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2017 by K. Rupp

Break down of DS (leakage current), **Moore's Law** (atom sized devices), **CS** (too much power)

Evolution towards heterogeneous systems with multi-core machines using co-processors (e.g., GPUs) and complex memory configurations

Computing in HEP is not business as usual anymore

Hardware evolution calls for a redesign of the computing model for HEP

- **Experiment software frameworks** will need to use heterogenous resources locally and remotely, including supercomputing centers and commercial facilities
- **Data Management Model** to handle data access, transfer, processing across a diverse set of computing systems
- **Adapt or re-engineer almost every piece of software**, including common software tools for event generation, detector simulation, end-user analysis, reconstruction algorithms
- **Portability tools** to avoid re-writing software for different computing hardware
- **Computing and software infrastructure for AI/ML** training and inference

Departure from stability of the past when the “same old software” would run faster and cheaper in future machines without adaptation or re-engineering

Research - to bridge the needed versus available resource gap and, development - to deliver production level software (heavy in labor - person power with rare and expensive talents)

S&C in HEP evolved to become an integral part of the measurement instrument

- **Not a "service" but an "element" of the "scientific apparatus" in HEP experiments/surveys**
- Complexity and physics content/impact of computing commensurable with that of detectors
- Exploit synergy between detector and software design

  Co-development, with simulation to design/optimize detectors and detector parameters optimized for best physics and computing performance

Main recommendation

We recommend the creation of a standing **Coordinating Panel for Software and Computing (CPSC)** under the auspices of DPF, mirroring the panel for advanced detectors (CPAD) established in 2012.

Promote, coordinate, and assist the HEP community on Software and Computing, working with scientific collaborations, grassroots organizations, institutes and centers, community leaders, and funding agencies on the evolving HEP Software and Computing needs of experimental, observational, and theoretical aspects of the HEP programs. The scope should include research, development, maintenance, and user support.

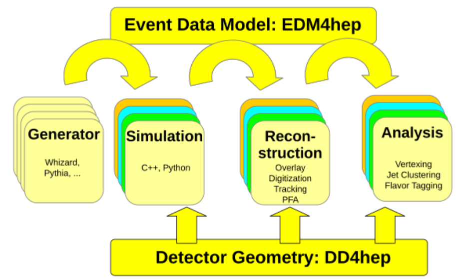
(There is also a recommendation for the CPSC to setup a study group on DEI in HEP computing – See backup slide for details.)

Common Software Stack

Key4hep: Turnkey Software Stack

Structured software stack integrating individual packages towards a complete data processing framework for HEP experiments

- Reduce overhead for adopting projects by sharing common components
- Easy to use for librarians, developers, users
- Functionality-complete: plenty of examples for simulation and reconstruction of detectors
- Preserve and adapt existing functionality into the stack, e.g., from iLCSoft, FCCSW, CEPCSW



Main ingredients

Event Data Model (podio/EDM4hep) (see **talk by T. Madlener**), Geometry Information (DD4hep), Processing Framework (Gaudi), Package manager (Spack)

G. Ganis, A. S 截屏 Key4hep: Progress Report on Integrations - CHEP 2023, May 11, 2023 3 / 15

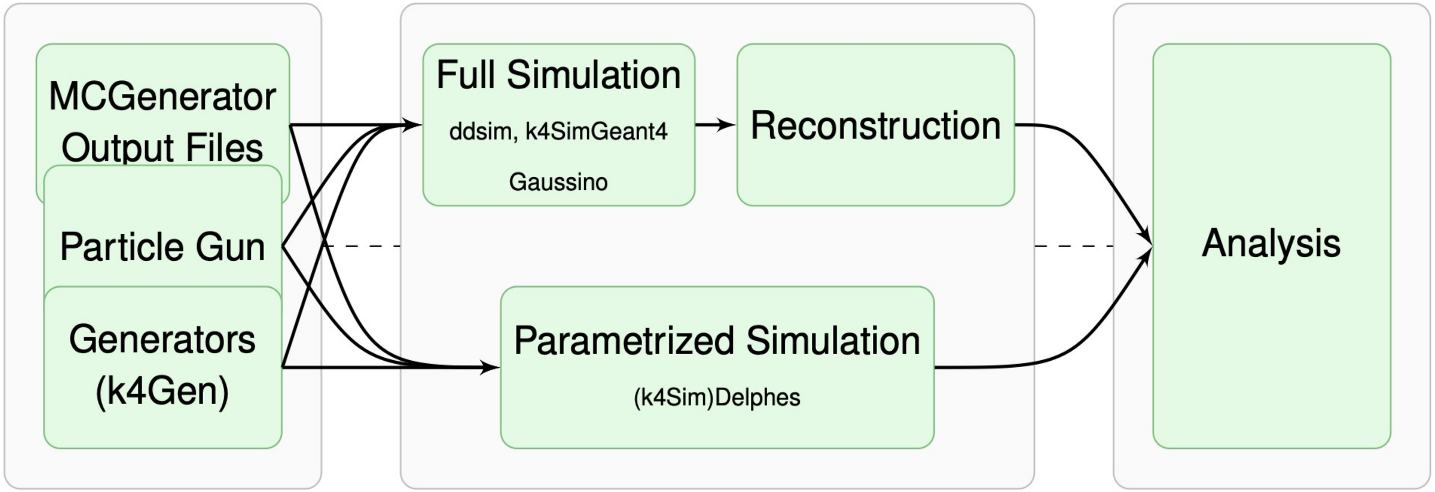
International Community

- Contributors/Interest from China, Germany, Italy, Americas, CERN; CEPC, CLIC, EIC, FCC, ILC, MuonCol

Key4hep

Simulation Integrations

- Key4hep allows to run fast parameterized simulation via Delphes, or Geant4 Simulation via DD4hep::ddsim (standalone) and k4SimGeant4 (Gaudi interface)
  - All solutions output data in EDM4hep format to be used in digitisation / reconstruction
- k4SimGeant4 essentially has the same goal as **Gaussino**
  - Adoption of Gaussino planned as a replacement for k4SimGeant4, aligning-with/adopting functionality from DD4hep::DDG4

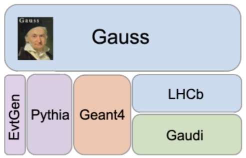


Gaussino

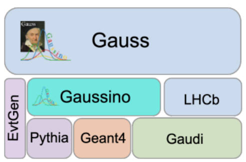
From Gauss to Gauss-on-Gaussino

LHCB-TDR-017

💡 **Introduce an experiment-independent layer!**



(a) Gauss current dependencies



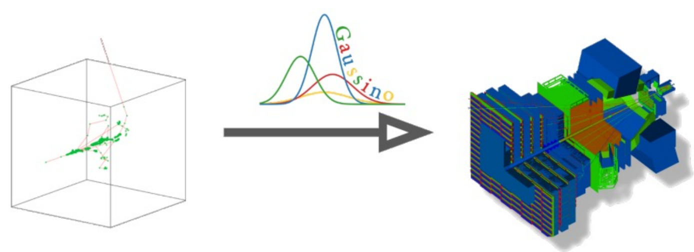
(b) Gauss-on-Gaussino dependencies

- Gaussino
  - new core simulation framework,
  - created by extracting experiment-independent components from Gauss,
  - ideal test bed for new developments,
  - idea came up in collaboration with the CERN SFT group / FCC,
  - 👉 **more on Gaussino** in the following talk!,
- Gauss-on-Gaussino
  - new version of LHCb simulation framework,
  - based on Gaussino's core functionalities,
  - adds LHCb-specific components and configurations,

Universal framework for simulations

🎯 use the **Gaussino** framework **for both**: test beams and final integration in the experimental setup!

- new core simulation framework to be used as a library or in a standalone mode,
- created by extracting experiment-independent components from Gauss,
- 👉 **more on Gauss-on-Gaussino for LHCb** in the previous talk!,
- in collaboration with the CERN SFT group / FCC,
- 👉 **more on Gaussino in Key4hep** in A. Salier's talk!,

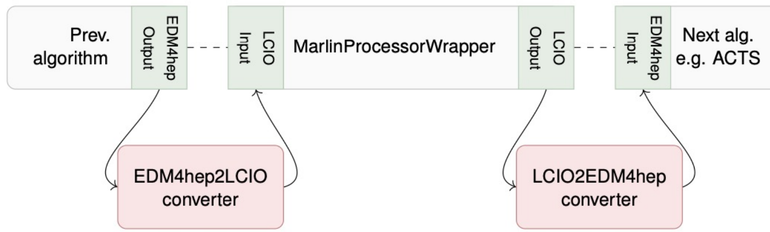


👉 **this talk** shows what **can already be done**!

Key4hep

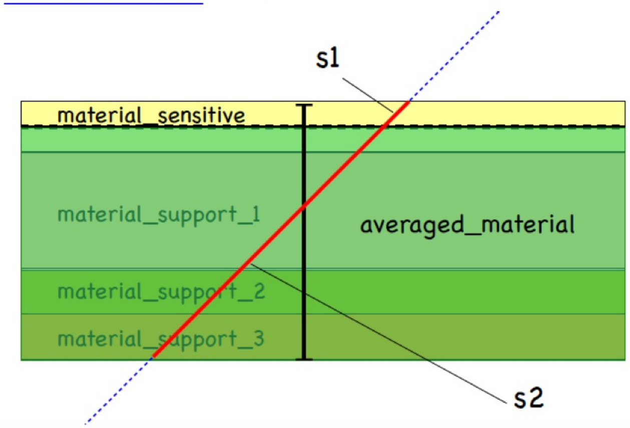
Track Reconstruction

- iLCSoft tracking algorithms available through the *k4MarlinWrapper* approach



- Integration of the ACTS tracking toolkit as thin Gaudi Algorithm *ongoing*:
  - Converting from EDM4hep to ACTS formats (see **P. Gessinger** talk)

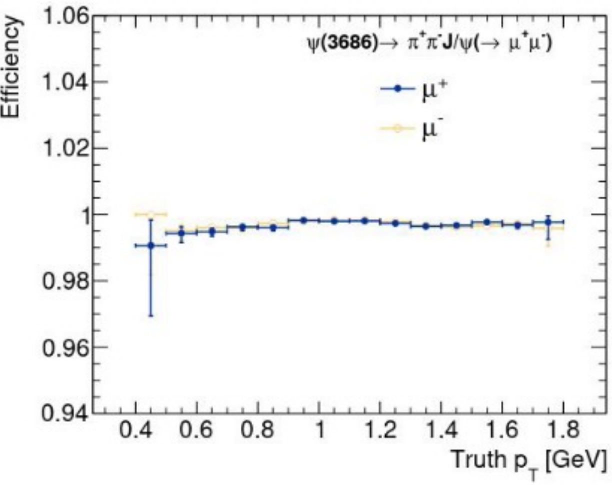
- Inject/add into ACTS surface information provided by `dd4hep::rec::Surface`
  - After the geometry instantiation, via DD4hep's plugin mechanism

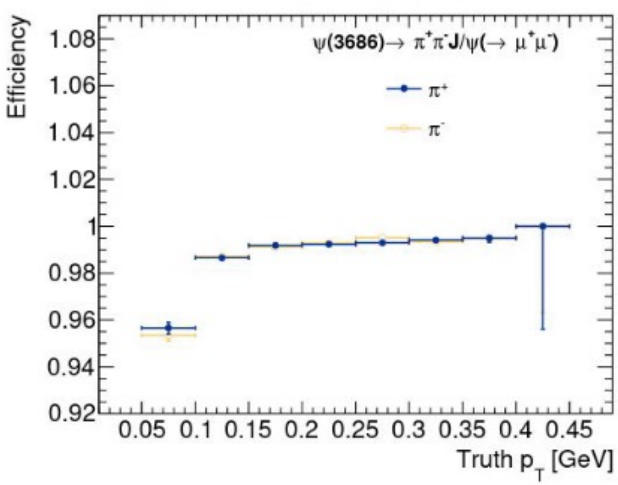


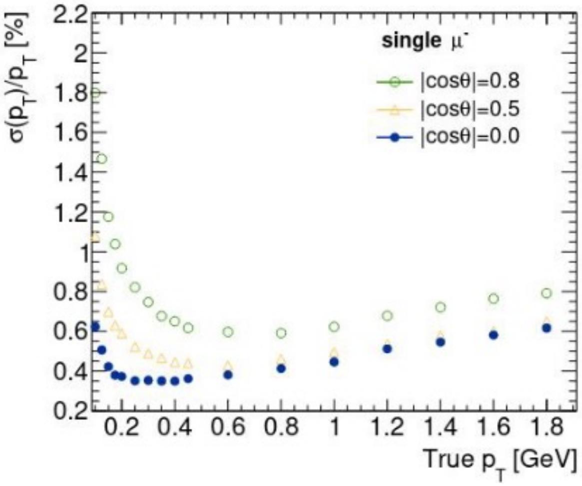
Implementation of ACTS for STCF

See our slides here

- First application and validation of ACTS for a drift chamber
- Promising tracking performance for STCF has been achieved
  - 94% tracking efficiency with p_T in [50, 100] MeV
  - $\sigma(p_T)/p_T < 0.5\%$ with $p_T = 1$ GeV, $\theta = 90°$ is achieved







Key4hep

Analysis with RDataFrame

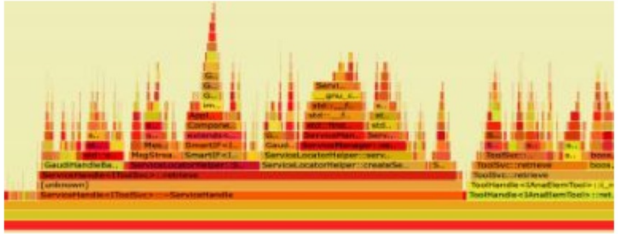
- EDM4hep data stored in ROOT Tree / RNTuple lends ideal candidate for analysis with RDataFrame
- Collection of tools in **FCCAnalyses**
- Example parts of the Higgs-Factory “Standard Candle” Higgs-Recoil analysis

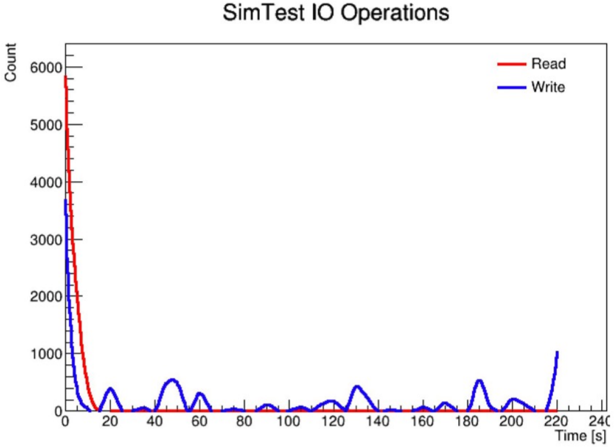
```
theDataFrame
# define an alias for electron index collection
.Alias("Electron0", "Electron#0.index")
# define the electron collection
.Define("electrons",  "ReconstructedParticle::get(Electron0, ReconstructedParticles)")
#select electrons on pT
.Define("selected_electrons", "ReconstructedParticle::sel_pt(10.)(electrons)")
# ...
.Define("zed_leptonic_recoil_m","ReconstructedParticle::get_mass(zed_leptonic_recoil)")
# create branch with leptonic charge
.Define("zed_leptonic_charge","ReconstructedParticle::get_charge(zed_leptonic)")
# Filter at least one candidate
.Filter("zed_leptonic_recoil_m.size()>0")
```

Key4hep

Testing

- The rate of changes and updates in the functionality requires monitoring and validation of performance
- Setting up continuous validation system able to monitor key performance indicators for any community (Detector Model) in Key4hep
- **Valprod**: toolkit to support building comprehensive validation jobs
  - Support CPU flame graph, I/O profiling
  - Integration with **HSF::prmon**





截屏

Key4hep

Summary & Outlook

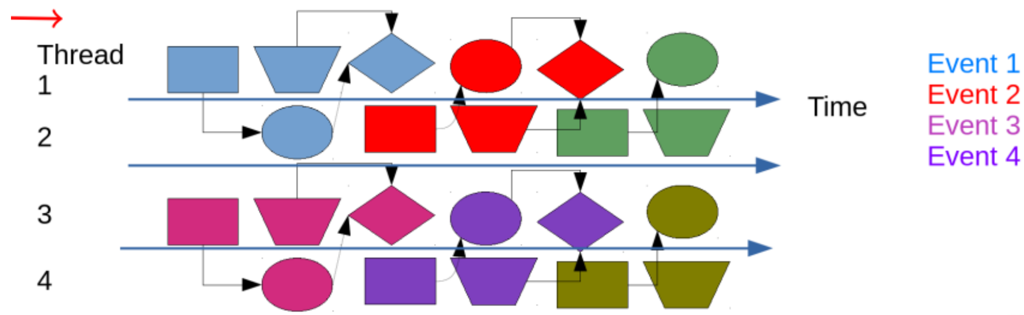
- Key4hep project is providing a common framework for future Higgs factories
  - Fully adopted by FCC, increasing adoption by CLIC, ILC, CEPC
  - Interest grown beyond the initial electron–positron collider communities (EIC)
  - New collaborators are always welcome
- Consolidation and expansion of the software stack to match the needs of the community is ongoing
  - By integrating new state-of-the art tools: PandoraPFA, ACTS, CLUE, Phoenix
  - Continuous Validation System to ensure everything keeps working together with high performance

截屏

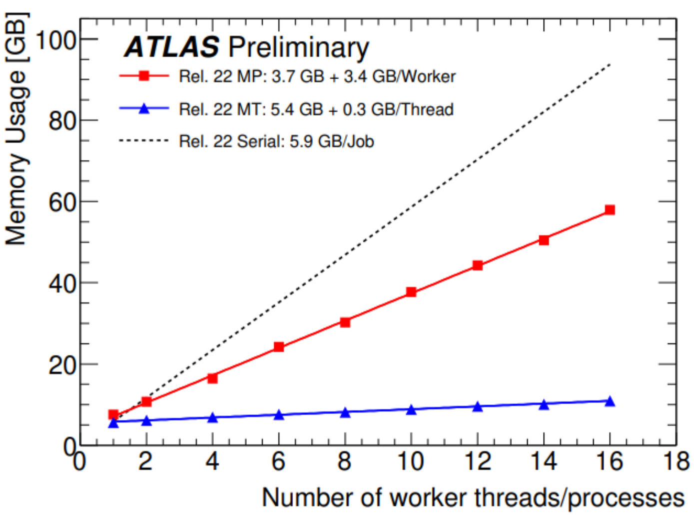
Framework

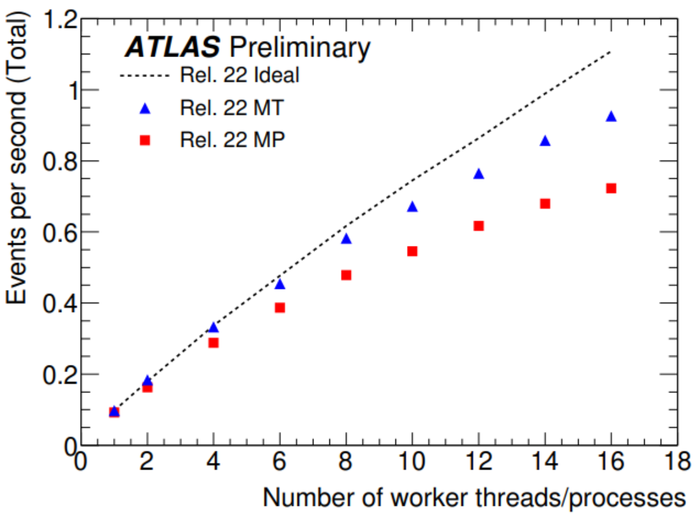
ATLAS: 从多进程AthenaMP到多线程AthenaMT

- 事例级并行 → 算法级并行
- 性能
  - 内存占用：显著降低
  - CPU：明显提升
- 一项持续数年的工作
  - 性能仍在继续优化中



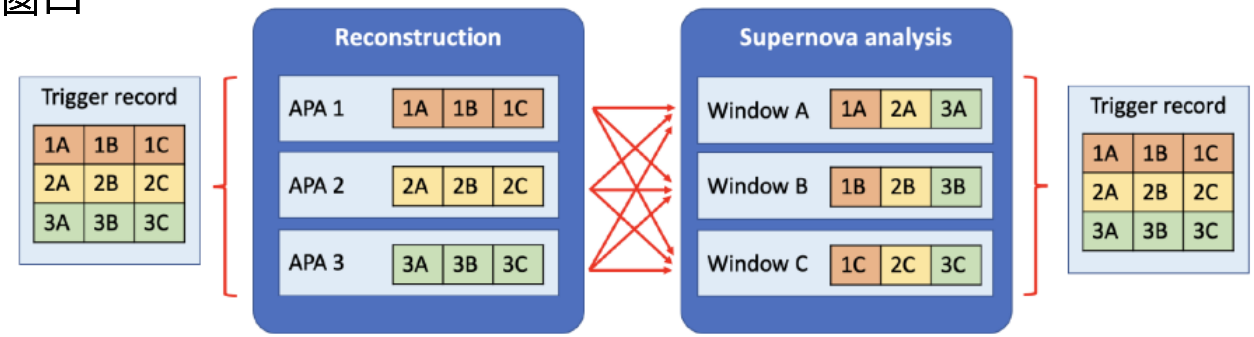
Different shapes: different algorithms; different colors: different events.





Meld: Exploring the feasibility of a framework-less framework

- DUNE：中微子实验
  - 先“事例”打散分开处理，再合并回“事例”
  - 滑动窗口



- 目前使用起源于对撞机实验的Art框架 → 探索性的Meld
  - 函数式编程思想，将数据处理过程抽象为高阶(high-order)函数

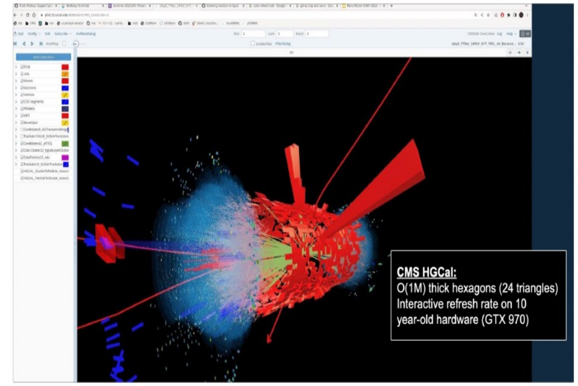
Supported construct	User function	
Transform (Map)	$f(a) \to b$	*Standard data-processing idioms*
Filter	$f(a) \to$ Boolean	
Monitor	$f(a) \to$ Void	
Reduction (Fold)	$f_c(a) \to c$	***For splitting and then combining events***
Splitter (Unfold)	$f_n(a) \to (d)_n$	
Zip	—	***For combining arguments to user functions***
Sliding window	—	*To do: **For sliding over adjacent events***

Data Preparation

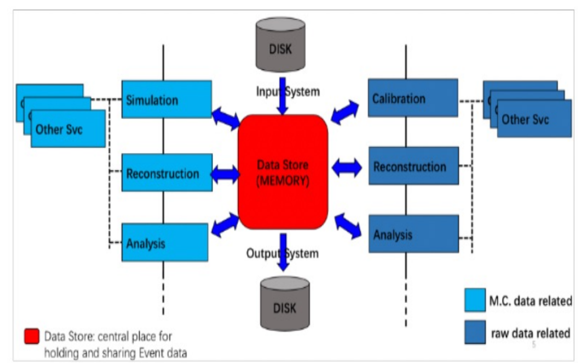
Large data volume in the current and future HEP experiments demands:

- Efficient data processing, transfer and storage
- Flexible and capable offline framework and infrastructure
- Improved event visualization

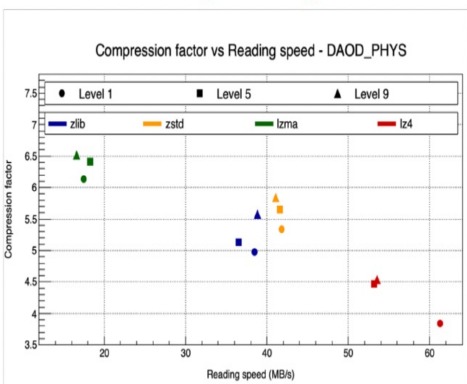
ROOT-EVE based CMS HGCal Display



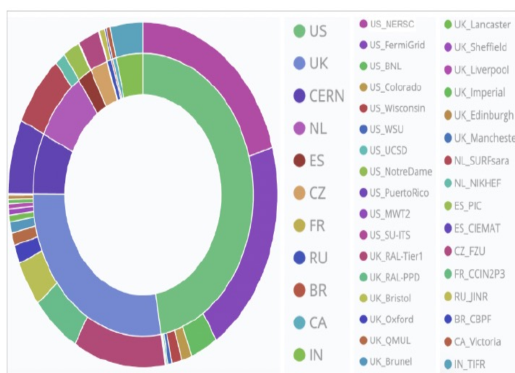
SNiPER Framework developed for JUNO



ATLAS data compression performance

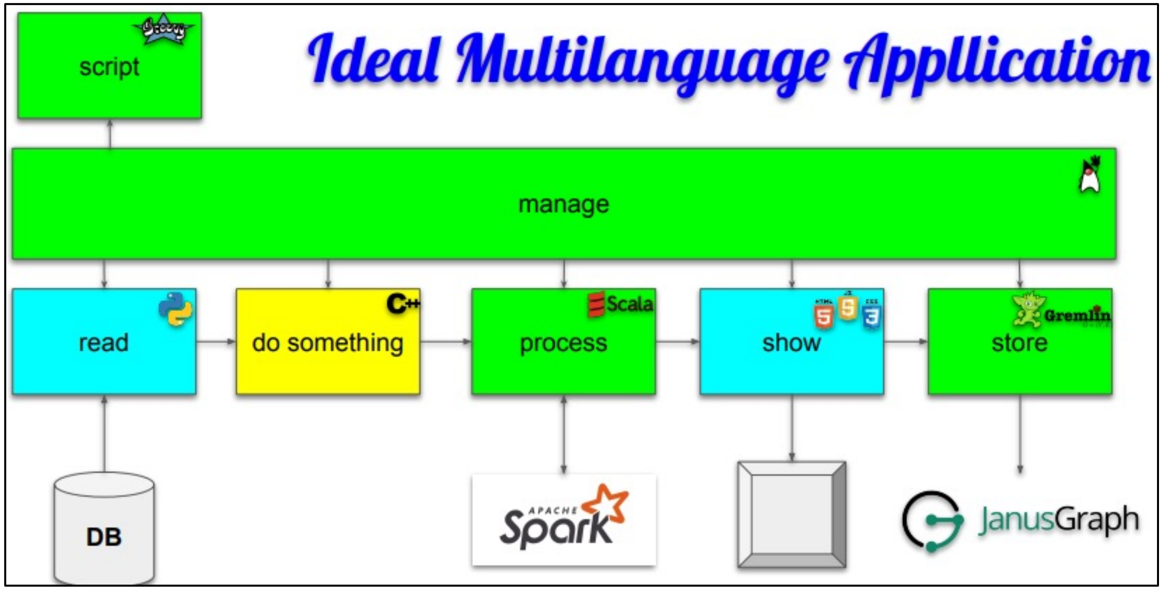


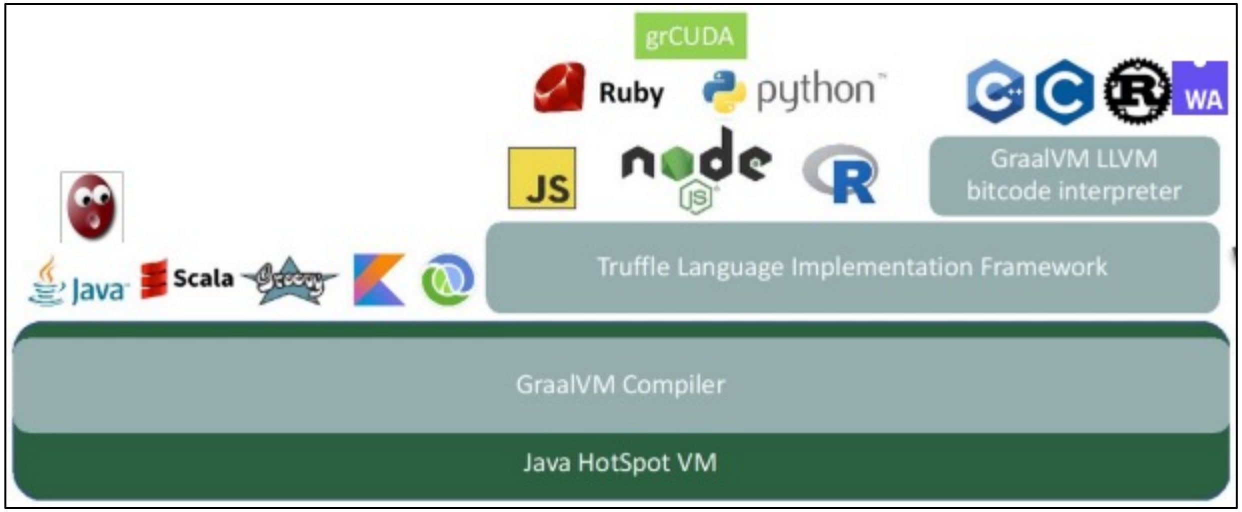
Grid job locations for DUNE data processing



Multilanguage Frameworks

- 功能分步，软件插件化
  - 黑盒子，外部无需知道内部细节（包括实现的语言）
  - 无缝衔接
- 使用合适的语言或工具做合适的事情
  - Scala：并行计算
  - JavaScript：图形化
  - …





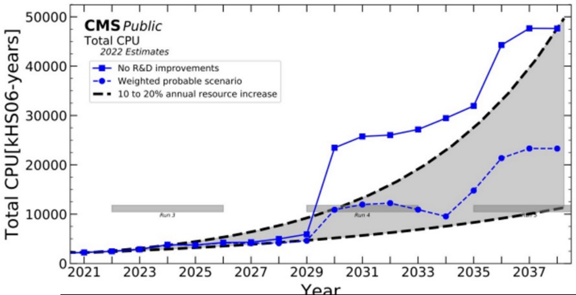
一种可能的方案：GraalVM

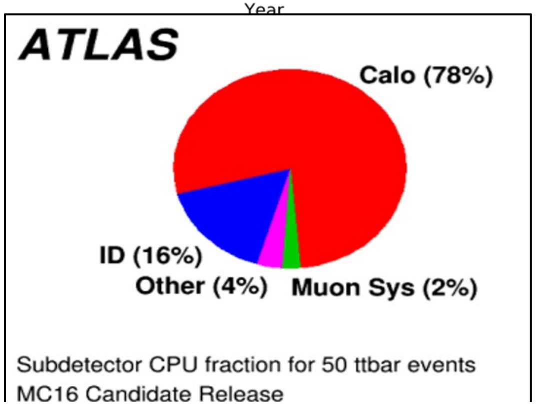
- 多种语言同时运行于一个环境空间中
- Oracle公司，社区版采用开源GPL License
- 已被Twitter等使用

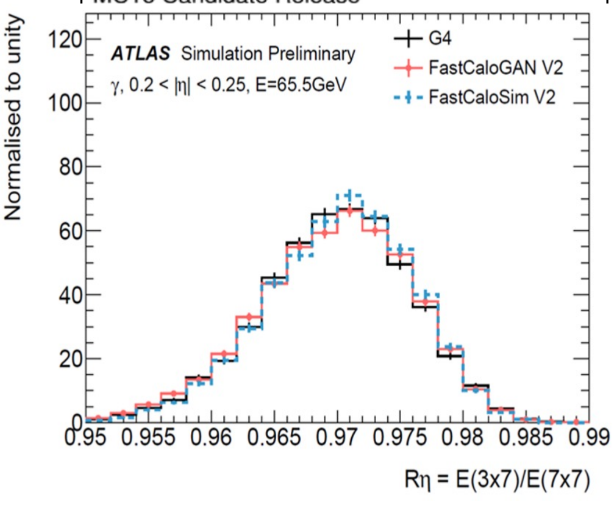
Machine Learning

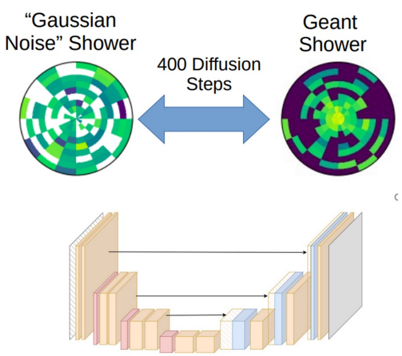
Fast Simulation（1）

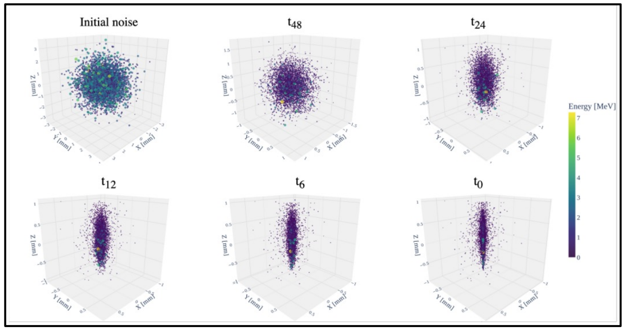
- 未来的 HL-LHC 实验将产生海量实验数据，需要产生与之相匹配的模拟数据。采用传统模拟方法将面临计算资源严重不足的问题。发展快速模拟方法具有重要科学意义
- 量能器的模拟占据了 Geant4 模拟的大部分资源，实现量能器的快速模拟能大大节约计算资源
  - ATLAS 已经将基于 GAN 的量能器快速模拟用于 Run2 MC 数据产生
  - 基于最新的机器学习技术的量能器快速模拟研究正在迅速开展中。例如基于 Diffusion 模型的 CaloDiffusion, CaloCloud 等





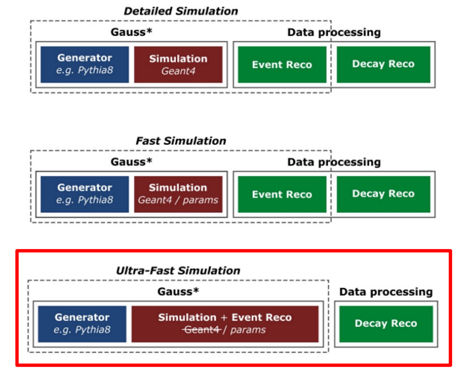


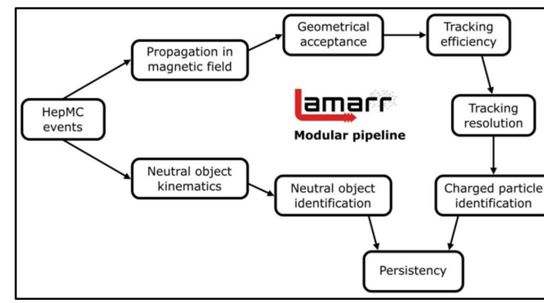


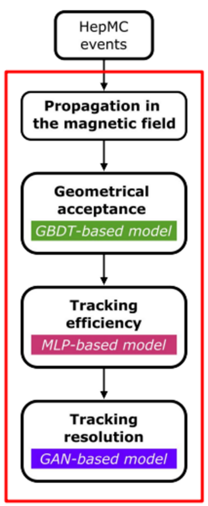


Fast Simulation（2）

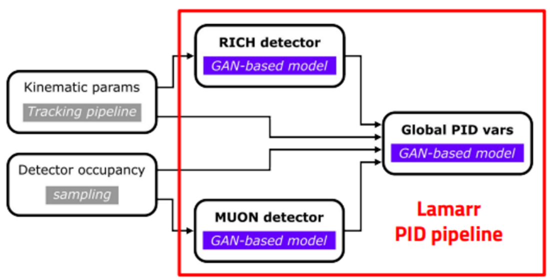
- End-to-end 的更加快速的模拟（Ultra-Fast Simulation）。跳过 Geant4 模拟，实现从 MC Particle 到用于物理分析的高级对象模拟
  - 例如 LHCb 的 Lamarr，CMS 的 FlashSim
- 基于机器学习方法（GBDT、MLP、GAN）实现对 tracking 重建效率（和分辨率）、PID、量能器（用于探测器性能研究）的快速模拟

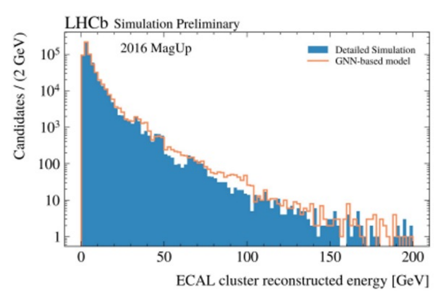


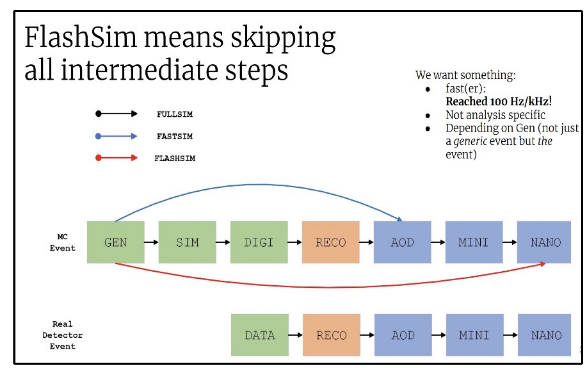




Lamarr
Tracking pipeline

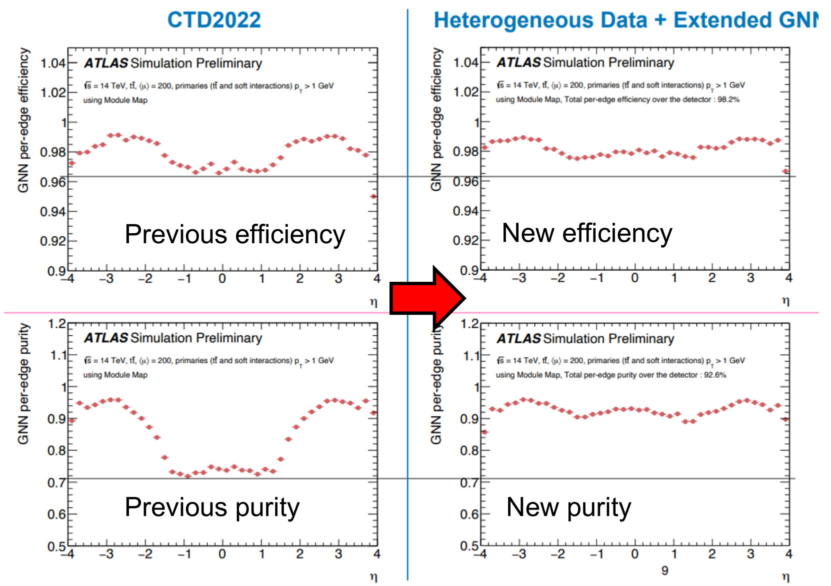




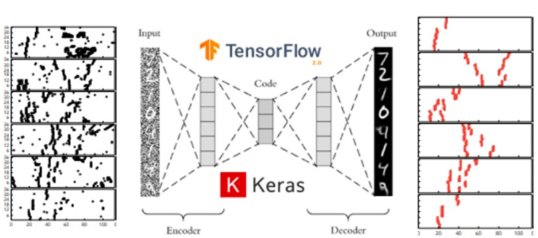


Track Reconstruction

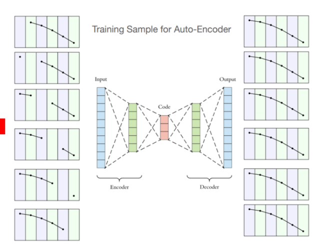
- BESIII 实验利用 GNN 进行噪声击中的排除，同时利用 DBSCAN 和 RANSAC 聚类算法实现径迹击中寻找，得到 promising 结果
- ATLAS 实验通过联合不同 tracker 子探测器（pixel+strip）以及对网络结构的优化大幅改善了 GNN 重建径迹的纯度



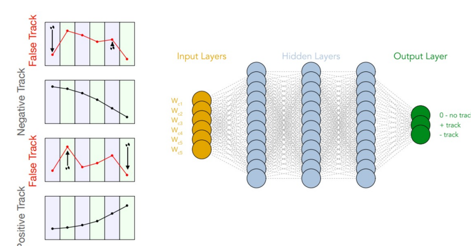
- Jefferson Lab 的 CLAS12 实验利用 Auto-Encoder 实现噪声击中的排除以及缺失径迹片段的补全，同时利用 MLP 加速径迹重建。最终提升径迹重建速度和性能



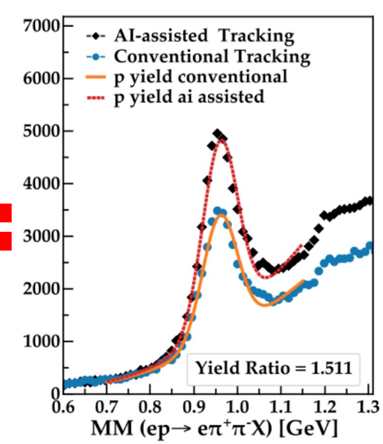
AE 噪声排除



AE 径迹段补全

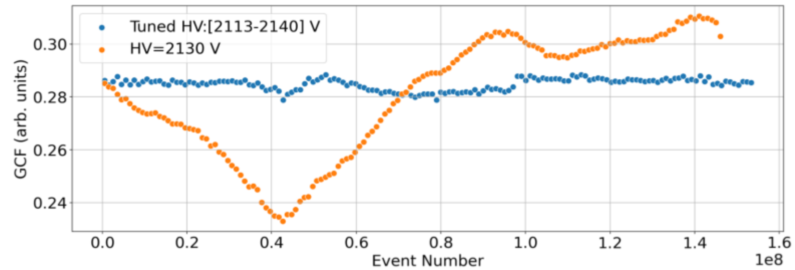


MLP 径迹重建

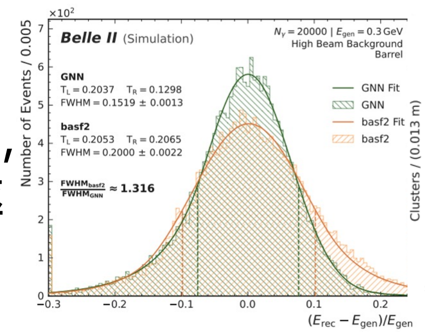


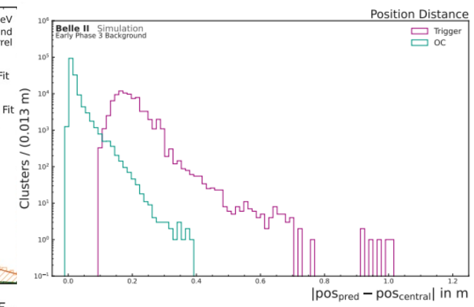
Online Application

- GlueX 实验利用 Gaussian Processes 方法根据探测器的温度、气压和束流状态在线调整漂移室的工作高压，提高取数质量

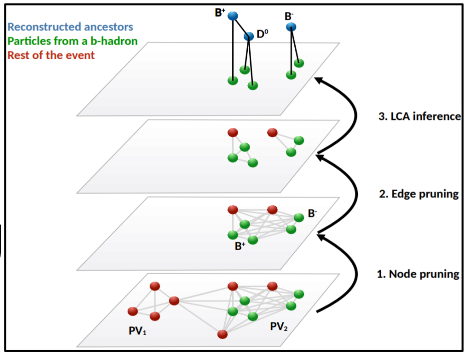


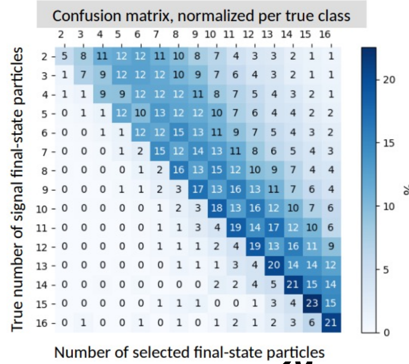
- Belle2 实验在 trigger 阶段通过 GNN 结合 Object condensation 聚合算法，有效提高了 Cluster 重建效率和分辨率（能量、位置）





- LHCb 实验为解决 HL-LHC 阶段在 trigger 方面面临的问题（重建速度、存储空间），开发了基于 GNN 的感兴趣末态粒子分类算法，得到 promising 结果





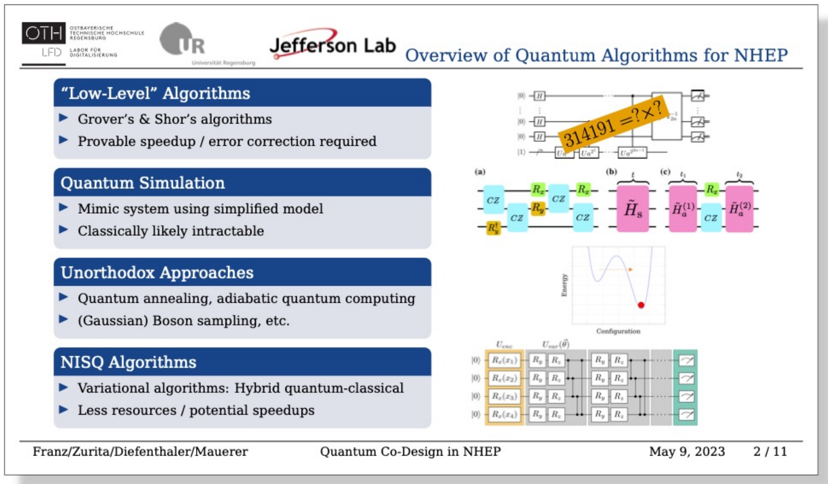
Quantum computing

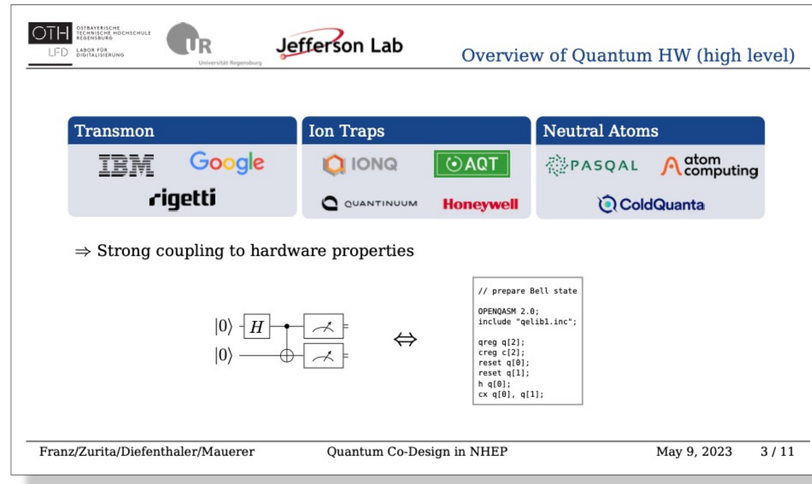
量子计算

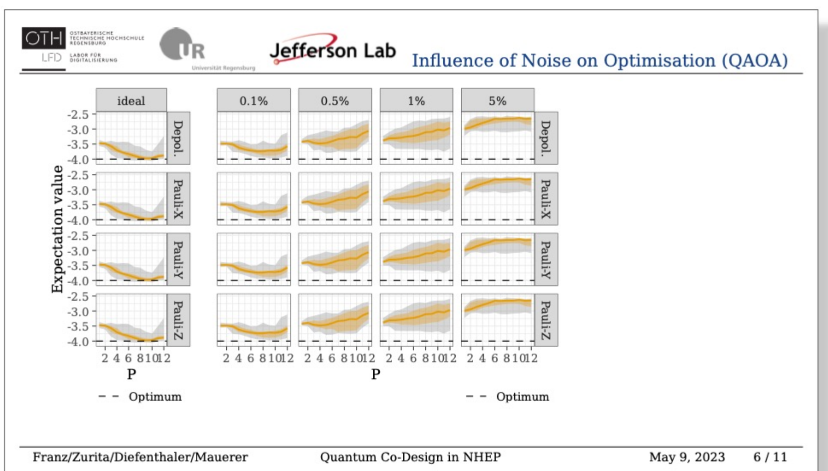
- CHEP 2023 – Track 12 (X): Quantum computing
  - 研究量子计算在高能物理理论、产生子、探测器模拟、重建和物理分析中的应用
- 1个Session, 共12个报告
  - Co-Design of Quantum Hardware and Algorithms in Nuclear and High Energy Physics
  - Towards a hybrid quantum operating system
  - Precise Image Generation on Current Noisy Quantum Devices
  - Application of quantum computing techniques in particle tracking at LHC
  - Connecting HEPCloud with quantum applications using the Rigetti platform
  - B Meson Flavour Tagging via Continuous Variable Quantum Support Vector Machines
  - First Measurements With A Quantum Vision Transformer: A Naive Approach
  - The Role of Data in Projected Quantum Kernels: the Higgs Boson Discrimination
  - Hybrid actor-critic scheme for quantum reinforcement learning
  - Improving Noisy Hybrid Quantum Graph Neural Networks for Particle Decay Tree Reconstruction
  - Symmetry Invariant Quantum Machine Learning models for classification problems in Particle Physics
  - Pion/Kaon Identification at STCF DTOF Based on Classical/Quantum Convolutional Neural Network

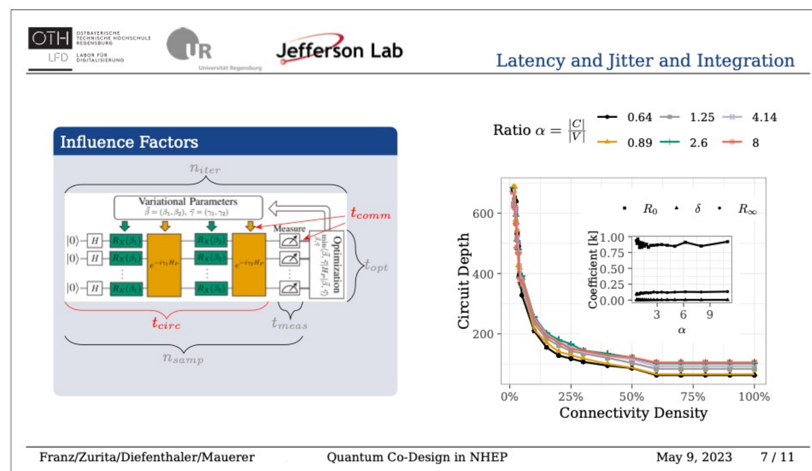
量子计算Highlight（I）

❖ 量子硬件与算法的协同设计



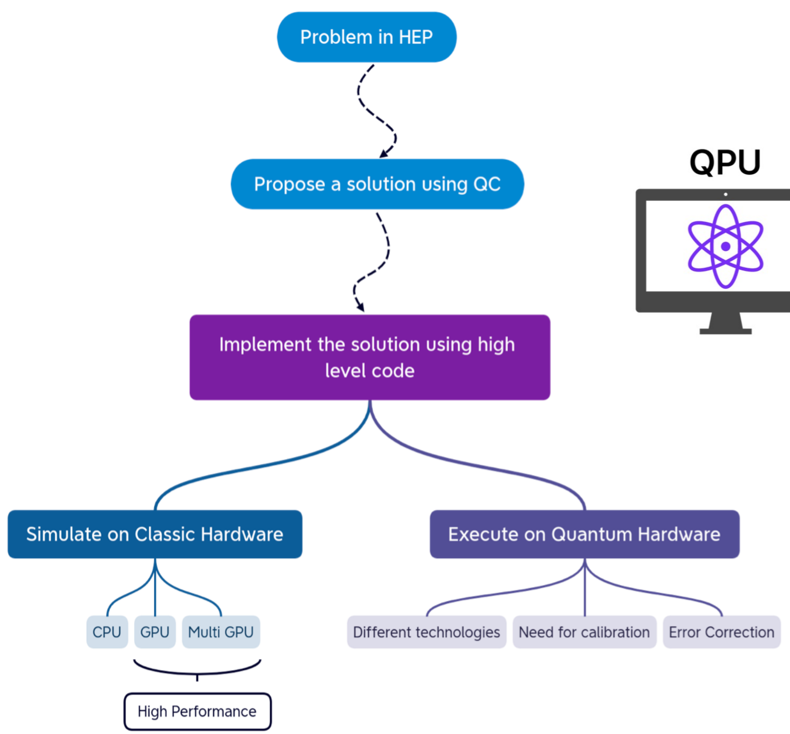




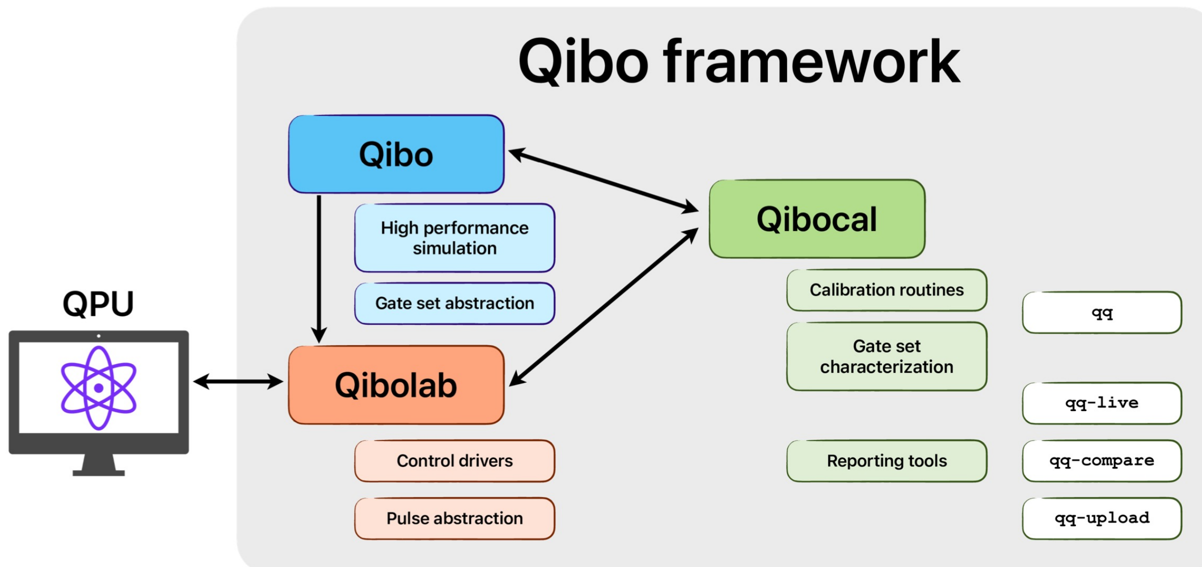


量子计算Highlight（II）

- Qibo framework: 量子计算“操作系统”



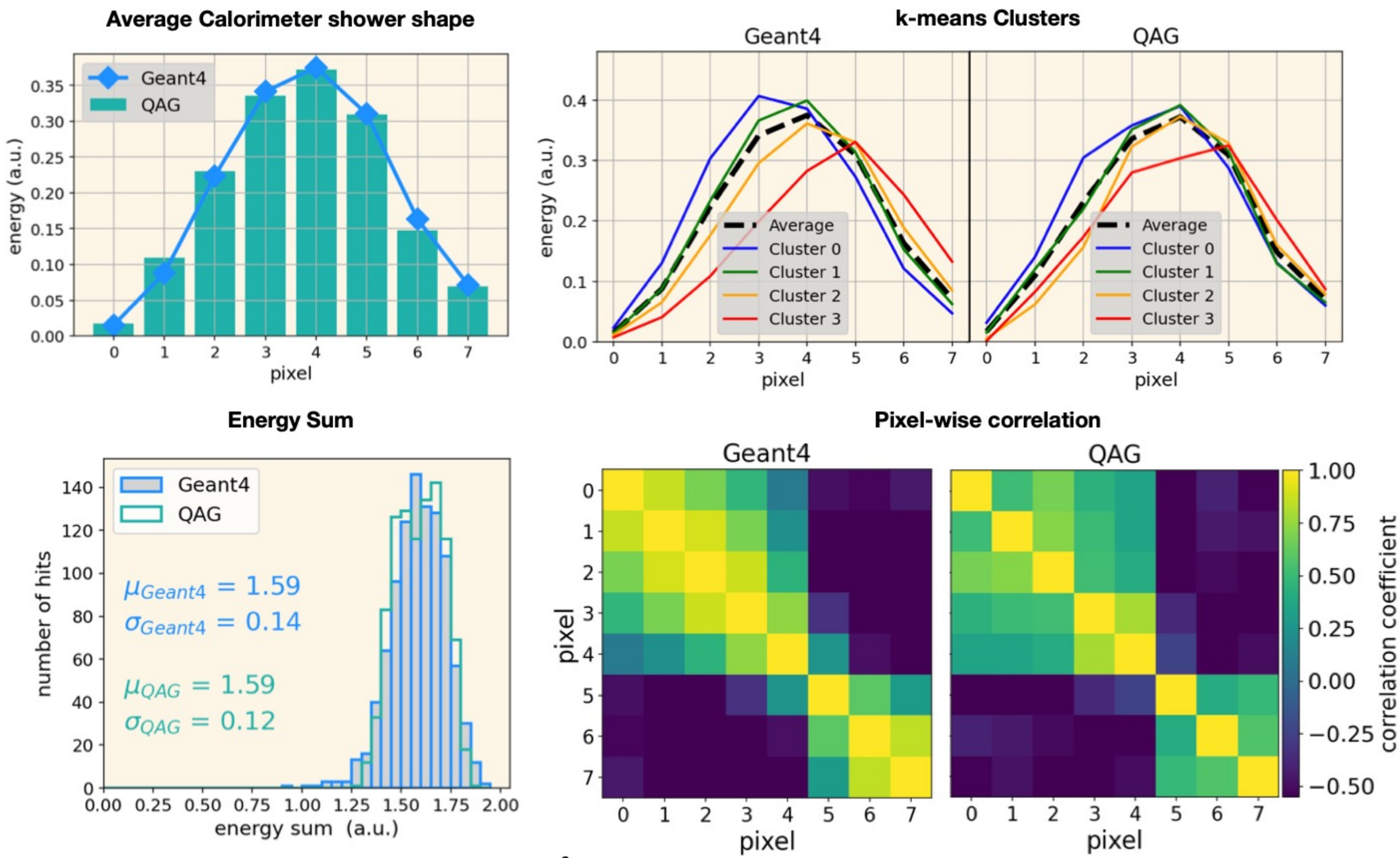
Is it possible to create from scratch a framework for all of this?



提供量子计算框架
实现线路模拟、后端连接等功能

量子计算Highlight（III）

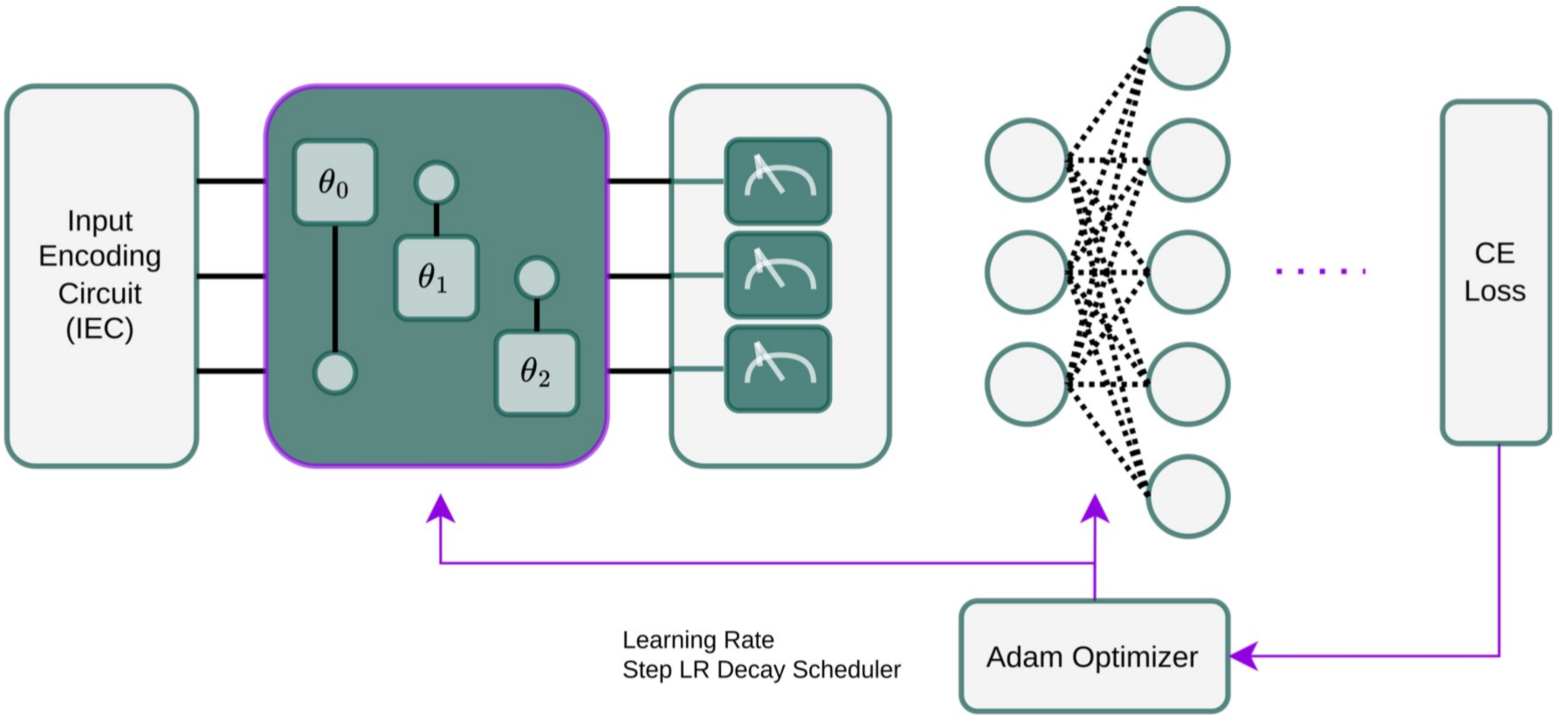
- 量子机器学习
  - Quantum Angle Generator：量能器快速模拟



量子计算Highlight（III）

❖ 量子机器学习

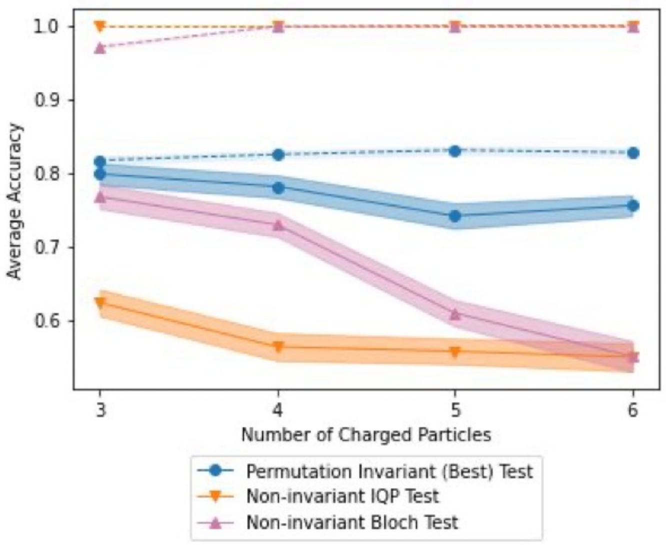
- Quantum GNN：寻迹算法、粒子衰变树重建



量子计算Highlight（IV）

❖ 量子机器学习

- Quantum Support Vector Machine：Flavor Tagging、PID



Weightings in data:

3 particles : 20%

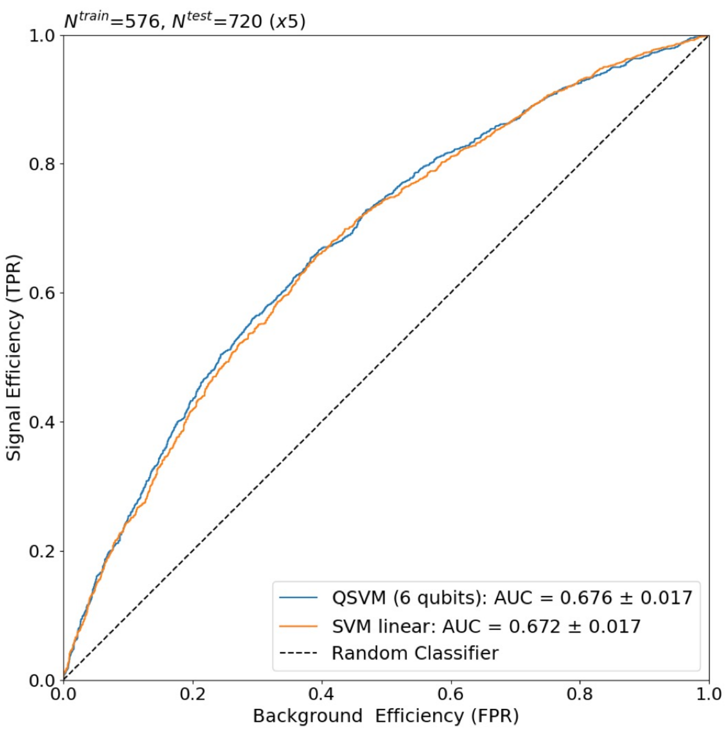
4 particles : 14%

5 particles : 18%

6 particles : 12%

Weighted Averages:

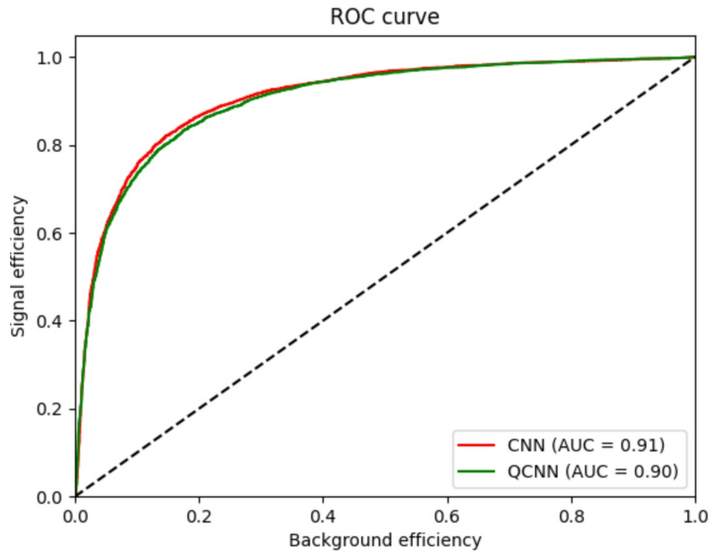
Permutation Invariant = 0.77
Non-invariant = 0.67

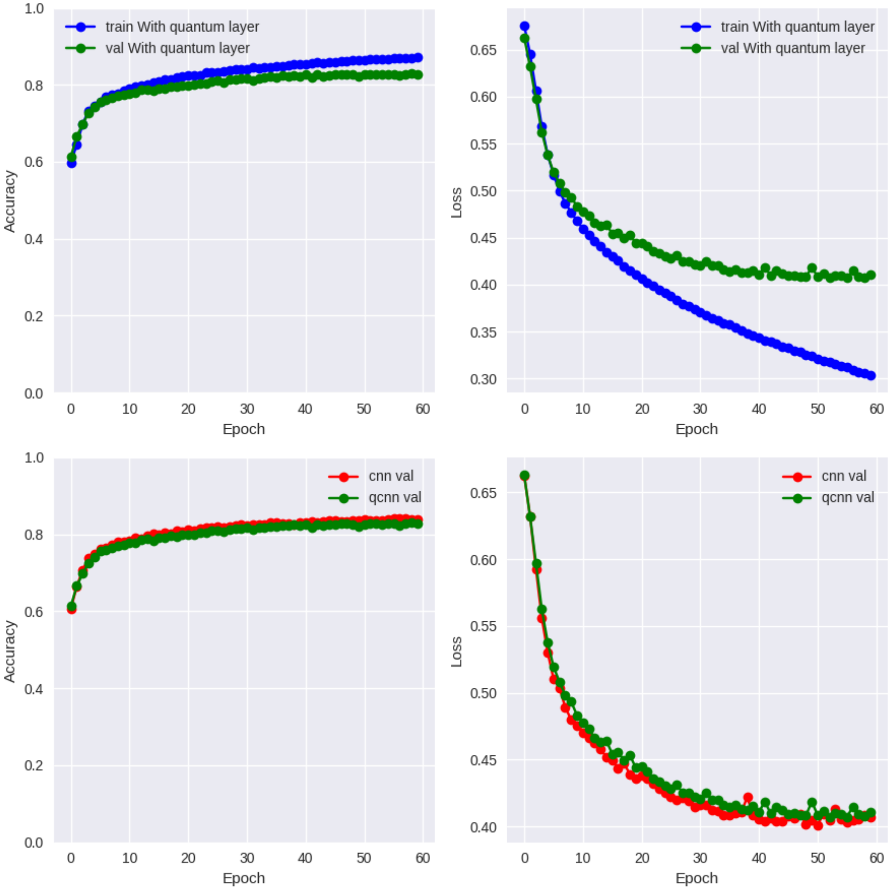


量子计算Highlight（IV）

❖ 量子机器学习

- Quantum CNN：π/K identification at STCF



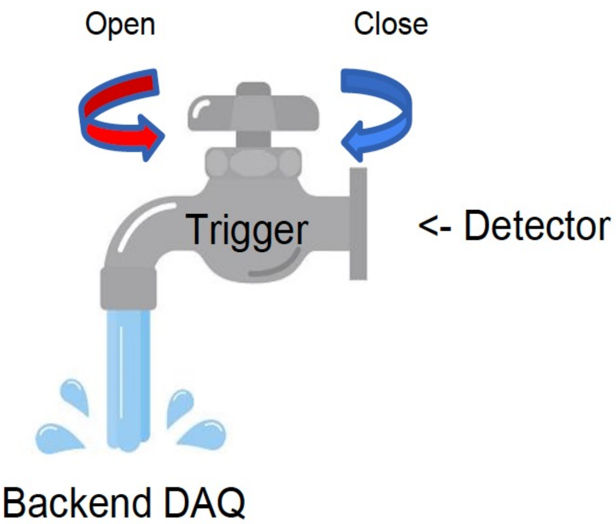


Heterogeneous Computing and Accelerators

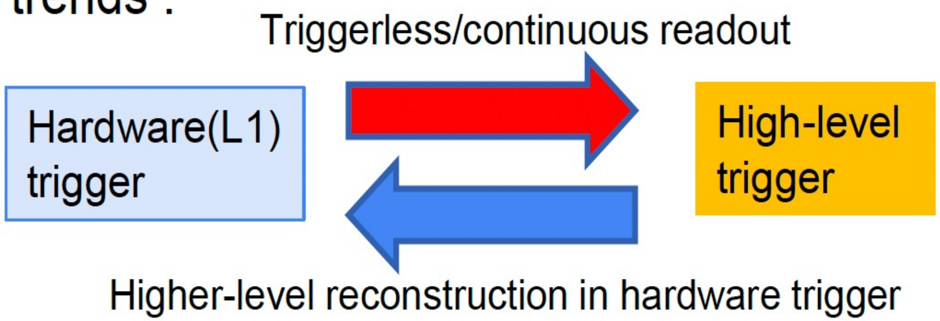
Trigger scheme

Two very important but basically conflicting demands for Trigger

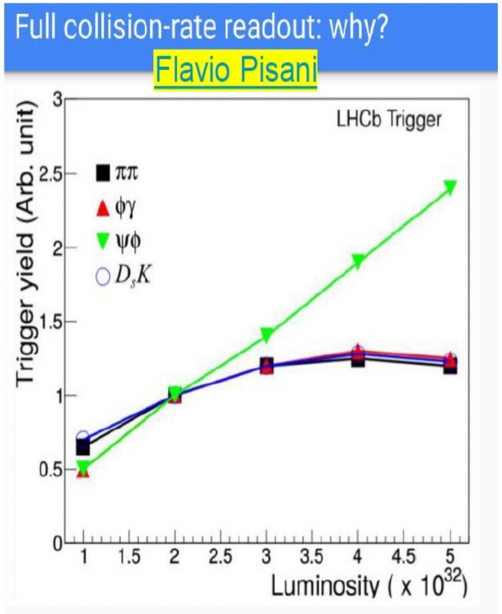
- Decrease throughput to backend DAQ
- Keep trigger-efficiency high



Two trends :

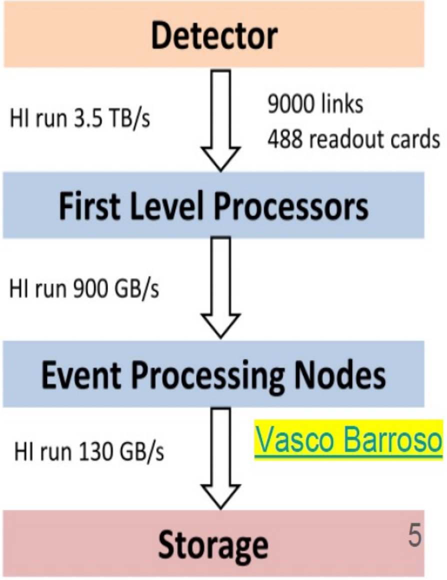


"One year of data taking": Triggerless/streaming readout



- Triggerless DAQ in LHCb
  - The system has been successfully used for the first part of Run3 !
  - Development : Implementing trigger for Long-lived particle detection (short track and displaced vertex)
- New ALICE DAQ system (O2/FLP) for Run3
  - Reconstruct TPC data in continuous readout in combination with triggered detectors.
  - Excellent initial performance, quite promising for Run 3

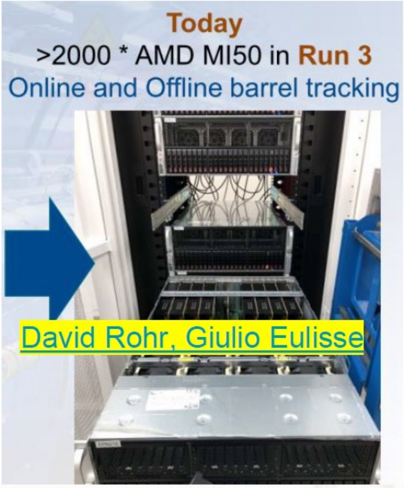
ALICE data-flow

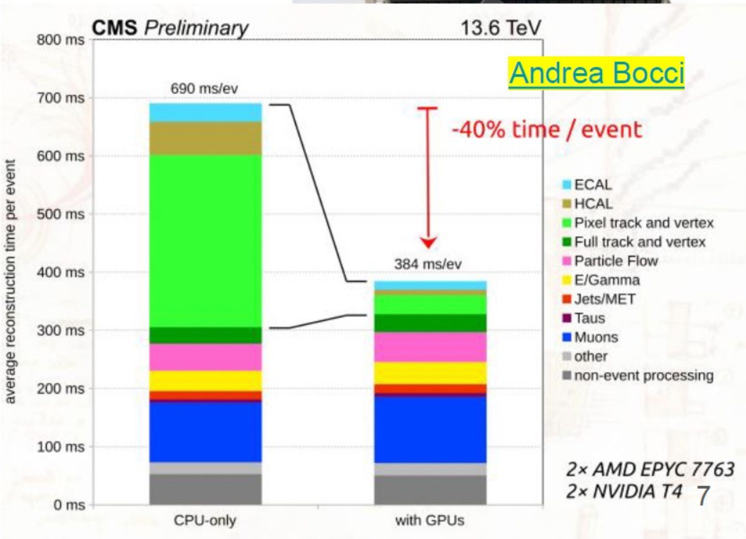


Accelerated online Computing : GPU

- ALICE Run 3: GPU for online (&offline) reco acceleration.
  - Without GPUs, more than 2000 64-core servers would be needed for online processing!
- CMS Run 3: 40% of reconstruction accelerated by GPUs
  - Achieve full performance portability with Alpaka

GPU in ALICE DAQ

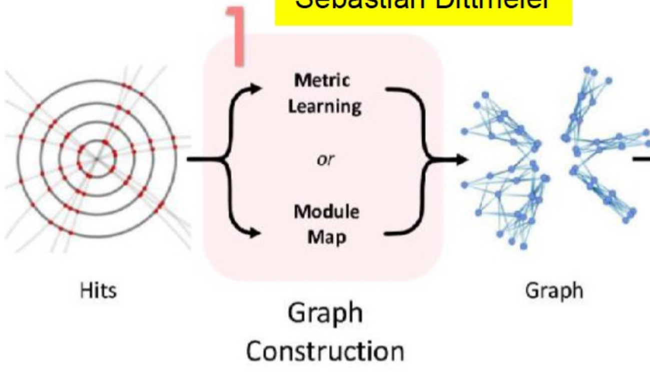




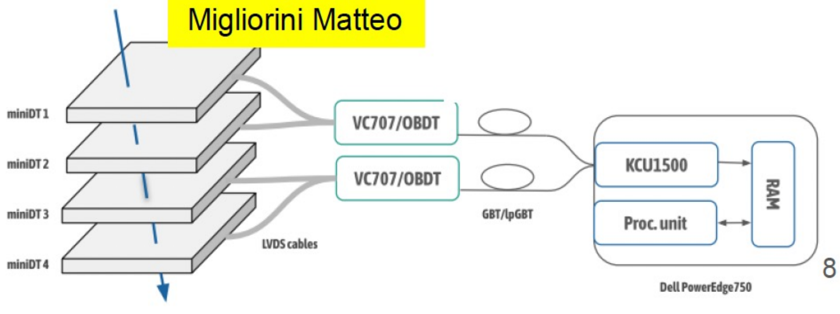
Accelerated online Computing : FPGA

- GNN in ATLAS event-filter for HL-LHC
  - FPGA resource constraints : Quantization + Pruning was used in the study
- Triggerless DAQ with Anomaly detection of machine learning
  - It sounds interesting if we can keep the main DAQ running and adding a simple triggerless DAQ system for exotic-event search, for example.

Sebastian Dittmeier



Migliorini Matteo



Sustainable and Collaborative Software Engineering

可持续与合作的软件工程

Topics

Sustainable Languages and Architectures

Sustainable CI and Build Infrastructure

Glance and Web based applications

Sustainable Analysis

MISC: MonteCarlos, Infrastructure and Simulation

Sustainable Frameworks

A total of 33 talks in 6 sessions

Track 5

A Theme for this CHEP: Increasing adoption of open source tools outside of HEP & NP
Theme of this Track: Sustainability through sharing of common tools

Fri 12th May Plenary Session - Conference Highlights: Track 5

Liz Sexton-Kennedy, Track 5 Highlights

持续集成与测试

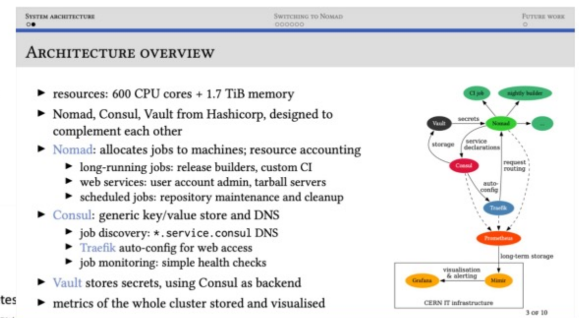
- 容器编排系统Kubernetes已经成为各个实验首选的基础架构
  - CERN IT、ALTAS、ALICE、JUNO
- GitLab/GitHub成为项目持续集成的新方式
  - YAML + Git

Sustainable CI and Build Infrastructure

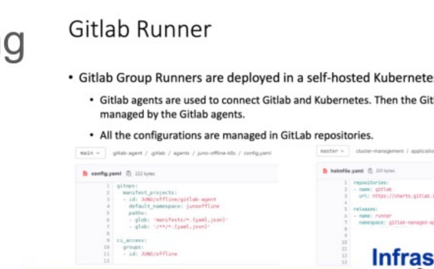
A common trend across the experiments is orchestration & containers using kubernetes or nomad

Jenkins still heavily used.

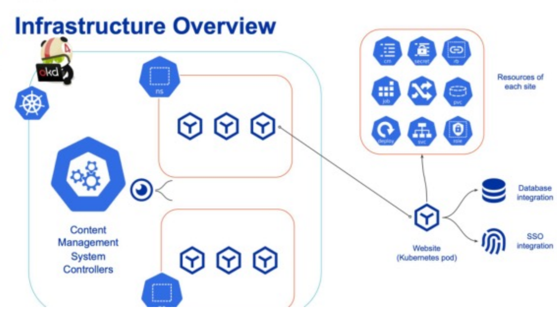
Gitlab / Github actions new way of defining builds.



ALICE is using Hashicorp Nomad, Vault and Cosul



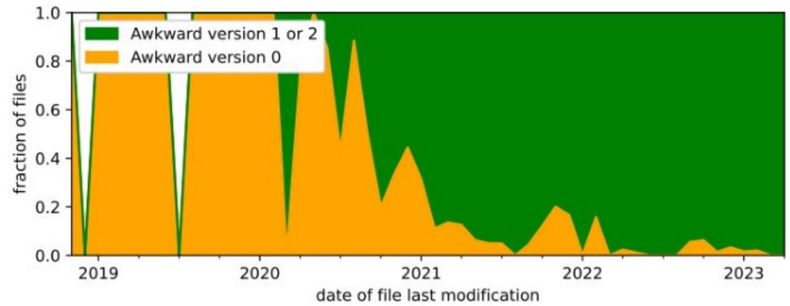
Juno has modernized it's software practices following HSF recommendations



CERN web services have been automated and more configuration is delegated to users

可持续的分析

- 采用Git作为版本控制，按照软件开发的模式开展分析
- 利用YAML简化用户使用的界面，同时更易管理和追踪。



Sustainable Analysis

"Analysis of physics analysis"

- Idea to learn from Git repositories. Study limited to CMS
- We can learn things that are useful for software library maintenance
  - user adoption of new versions
  - most common function-call patterns
  - decide if and when a feature can be deprecated
  - discover which libraries are being used together, maybe motivate integrations

LbMCSubmit:

- New flexible & scalable request submission system for LHCb simulation
- Based on specifications in YAML, with review, CI test, then full submission

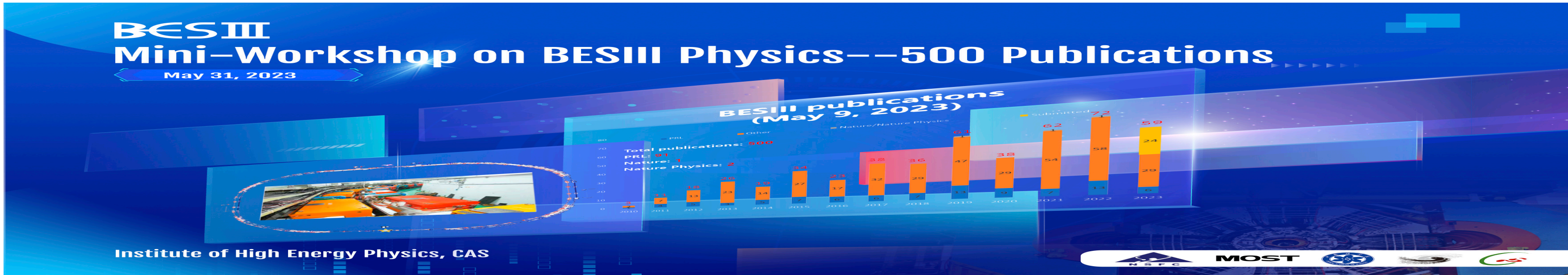
Simulation data quality in LHCb now integrated with DQ monitoring web-based tool

```yaml
sim-version: 09
name: Ds2KKpi
inform:
  - auser
  - firstname.surname@cern.ch
WG: Charm

samples:
  - event-types:
      - 23103005
      - 23103006
    data-types:
      - 2012
      - 2016
    num-events: 100_000
```

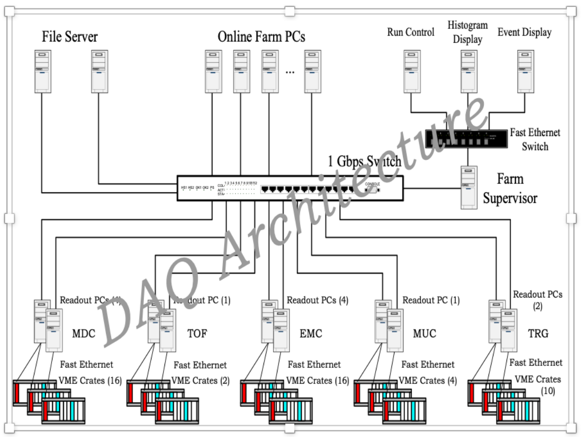
Summary

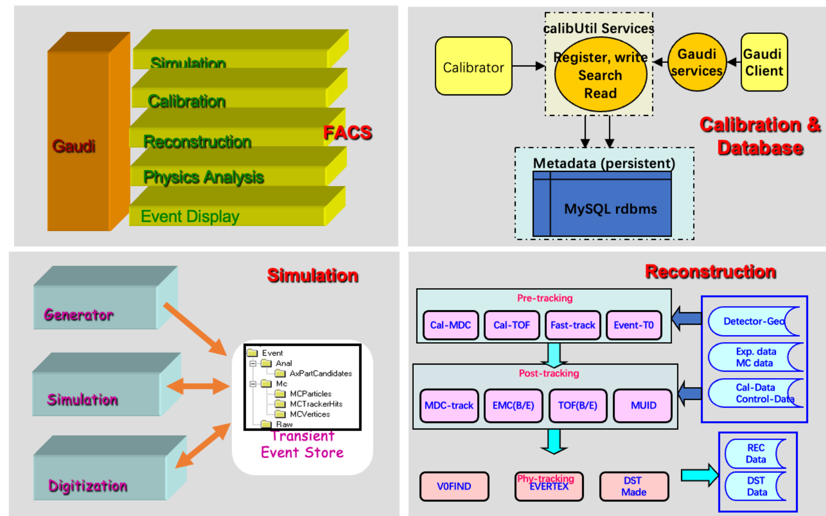
- Hardware drives redesign of the computing and software of HEP
- Recapped the partial of the highlights of CHEP2023
  - Common Software Stack
  - Framework
  - Machine Learning
  - Quantum computing
  - Heterogeneous Computing and Accelerators
  - Sustainable and Collaborative Software Engineering
- Lots of related works are being under-development in China and will be covered by the following talks.



DAQ and Offline

From Yifang's Talk





- Led by Prof. Kejun Zhu
- specification：~ 50Mb/s, 4000 Hz, 10 ×B-factory, 1000 × BESII
- Online monitoring, display and control

- Led by Prof. Weidong Li
- CMT based BESIII software development and management
- GAUDI based software framework
- GEANT4 based Monte Carlo simulation
- MYSQL based calibration and database

Thanks and Congratulations to people who ever made contributions to BESIII Offline Software!

Thanks for you attentions!