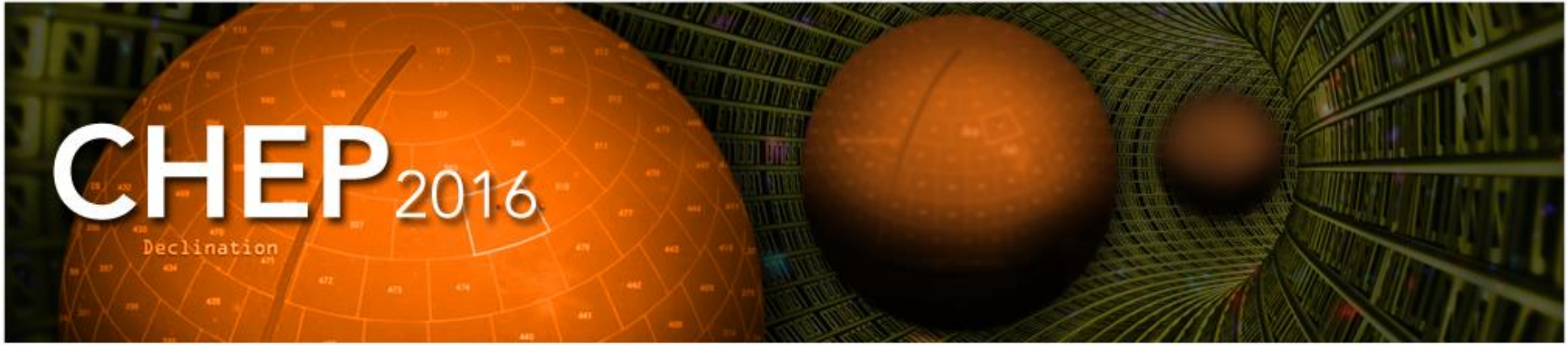


22nd International Conference on Computing in High Energy and Nuclear Physics, Hosted by SLAC and LBNL, Fall 2016

Track 5: Software development Highlights

Tina Cartaro

for the Track 5 conveners: Alberto Aimar, C.C., Florian Uhlig
and with contributions from the session chairs

Track 5 Sessions

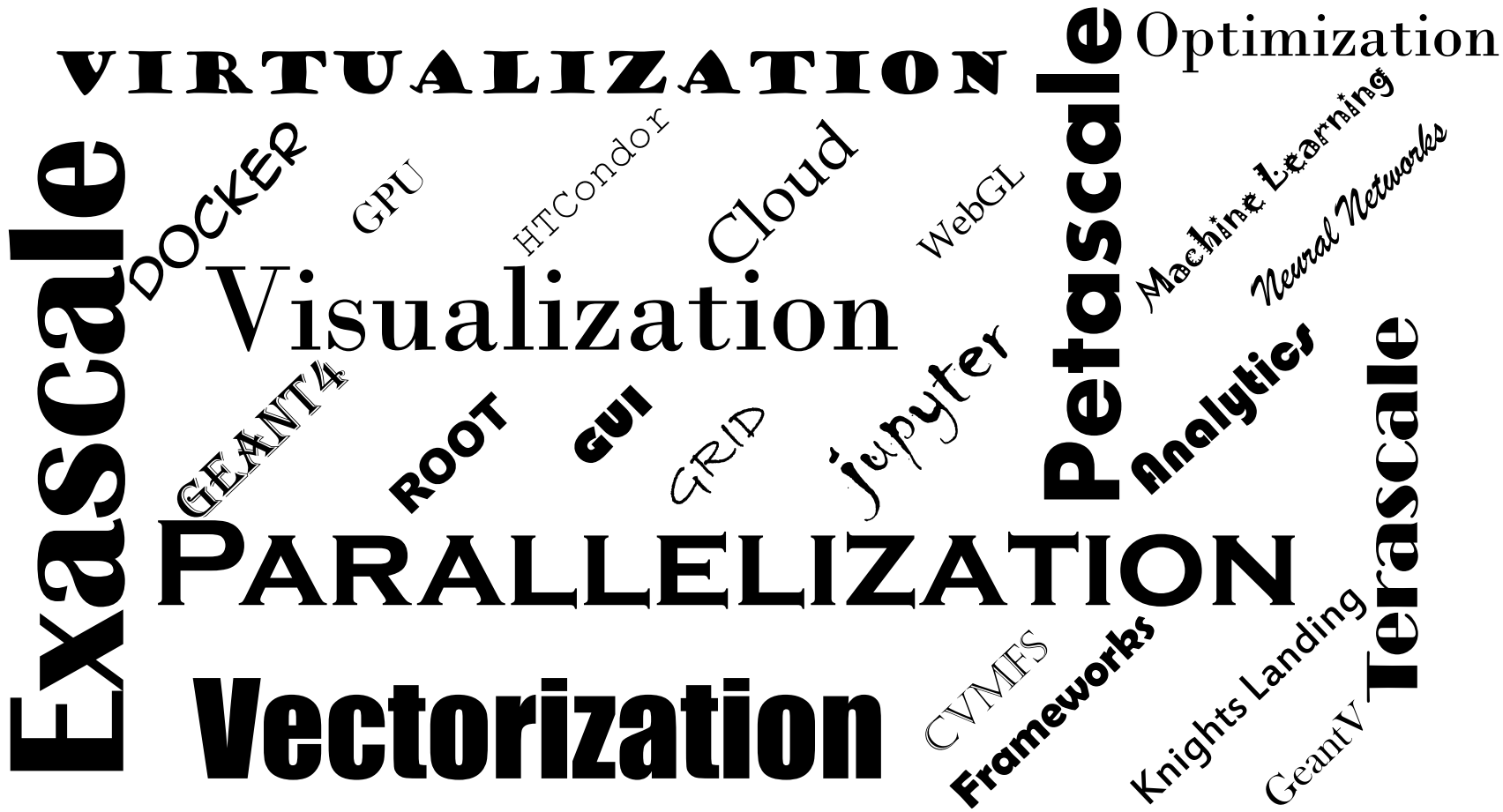
- 42 talks split in 7 sessions very roughly organized by topic
- 38 poster contributions in the 2 poster sessions
- Track 5 charge:
  - Software development process and tools; analysis tools and techniques; algorithms in the software development; visualization technology; frameworks for event processing; event data models; processor architectures; vectorization and parallelization; programming techniques and tools; software testing and quality assurance; configuration management; software build, release and distribution tools; documentation.

5.1 Physics application	5.2 ROOT	5.3 Performace, metrics, etc	5.4 Processors and architectures	5.5 Software Development	5.6 Visualization	5.7 Big Data
Chair: Steffen Luitz (SLAC)	Chair: Andreas Petzold (KIT)	Chair: Jakob Blomer (CERN)	Chair: Malachi Schram (PNNL)	Chair: Alberto Aimar (CERN)	Chair: Andrea Dotti (SLAC)	Chair: Marcus Ebert (U. of Edinburgh)

An impressive Wealth of Contributions

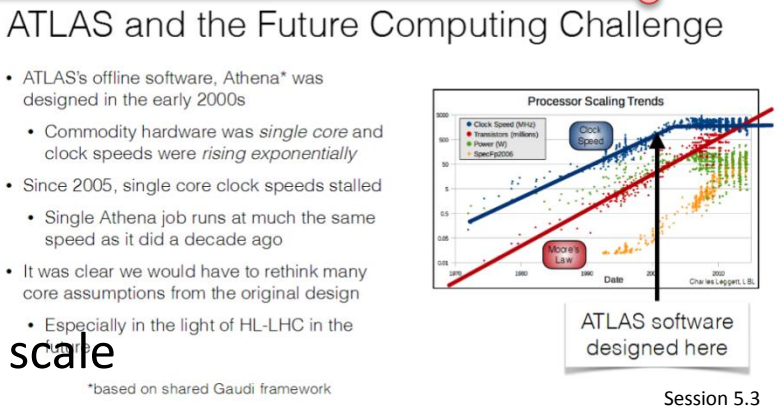
61 - Model-independent partial wave analysis using a massively-parallel fitting framework	Liang Sun et al.
100 - PODIO - Applying plain-old-data for defining physics data models	Benedikt Hegner et al.
237 - Tracking Machine Learning Challenge	David Rousseau et al.
552 - Using computing models from particle physics to investigate dose-toxicity correl...	Karl Harrison et al.
554 - Deep-Learning Analysis Pipelines on Raw HEP Data from the Daya Bay Neutrino Experiment at NERSC	Mr. Evan Racah et al.
562 - Neutrino Identification With A Convolutional Neural Network in the NOvA Detectors	Adam Aurisano et al.
157 - Status and Evolution of ROOT	Axel Naumann
156 - ROOT and new programming paradigms	Philippe Canal et al.
110 - Optimizing ROOT's Performance Using C++ Modules	Vasil Georgiev Vasilev et al.
258 - Expressing Parallelism in ROOT	Danilo Piparo et al.
260 - The New ROOT Interface: Jupyter Notebooks	Danilo Piparo et al.
321 - New Machine Learning Developments in ROOT	Dr. Sergei Gleyzer et al.
502 - Exploring Compression Techniques for ROOT IO	Brian Paul Bockelman et al.
9 - RootJS: Node.js Bindings for ROOT 6	Dr. Marek Szuba et al.
77 - Identifying memory allocation patterns in HEP software	Sami Kama et al.
158 - Computing Performance of GeantV Physics Models	Soon Yung Jun et al.
149 - How To Review 4 Million Lines of ATLAS Code	Graeme Stewart et al.
222 - Application of econometric and ecology analysis methods in physics software	Mincheol Han et al.
229 - First results from a combined analysis of CERN computing infrastructure metrics	Dirk Duellmann et al.

62 - CERN openlab Researched Technologies That Might Become Game Changers in Software Development	Fons Rademakers
306 - Software Quality Control at Belle II	Timothy Gebhard et al.
316 - Design and Execution of make-like distributed Analyses based on Spotify's Pipelining Package luigi	Marcel Rieger et al.
393 - Accelerating Navigation in the VecGeom Geometry Modeller	Sandro Christian Wenzel et al.
413 - Machine Learning with TensorFlow as an alternative to TMVA	Prof. Martin Sevior et al.
436 - Parallel Monte Carlo search for Hough transform	Raul Cardoso Lopes et al.
114 - Events visualisation in ALICE - current status and strategy for Run 3	Jeremi Niedziela et al.
117 - An interactive and comprehensive working environment for high-energy physics software w...	Mr. Nils Braun et al.
216 - Event visualisation in ATLAS: current software technologies / future prospects and trends	Riccardo Maria Bianchi et al.
449 - A browser-based event display for the CMS Experiment at the LHC using WebGL	Thomas Mc Cauley
561 - Integrating Visualization Applications, such as ParaView, into HEP Software Framewo...	Adam Lyon et al.
470 - Everware toolkit - supporting reproducible science and challenge driven education	Alexander Tiunov et al.
80 - A Comparison of Deep Learning Architectures with GPU Acceleration and Their Applications	Dr. Jin Huang et al.
161 - Multi-threaded Geant4 on Intel Many Integrated Core architectures	Andrea Dotti et al.
484 - Investigations of Future Computing Platforms for High Energy Physics	Aritz Brosa Iartza et al.
525 - Challenges in Scaling NLO Generators to Leadership Computers	Taylor Childers et al.
349 - A programming framework for data streaming on the Xeon Phi	Sylvain Chapeland
360 - "Big Data" in HEP: A comprehensive use case study	Oliver Gutsche et al.
69 - Big Data Analytics for the Future Circular Collider Reliability and Availability Studies	Andrea Apollonio et al.
176 - XRootD Popularity on Hadoop Clusters	Marco Meoni et al.
231 - Hadoop and friends - first experience at CERN with a new platform for high throughput analysis steps	Dirk Duellmann et al.
215 - Big Data Analytics Tools as Applied to ATLAS Event Data	Ilija Vukotic et al.
263 - Developing and optimizing applications for the Hadoop environment	Prasanth Kothuri et al.


VIRTUALIZATION
Optimization
Exascale
DOCKER
GPU
HTCondor
Cloud
WebGL
Petascale
Machine Learning
Neural Networks
Visualization
GEANT4
ROOT
GUI
GRID
jupyter
Analytics
Terascale
PARALLELIZATION
Vectorization
CVMFS
Frameworks
Knights Landing
GeantV

The Path to the Next Level Up

- The CPU clock speed flat-lined years ago, the level of parallelization in hardware has increased, and the complexity of the HEP (and non-HEP) applications has grown. Even more growth is expected in the coming years together with the growth of the datasets scale

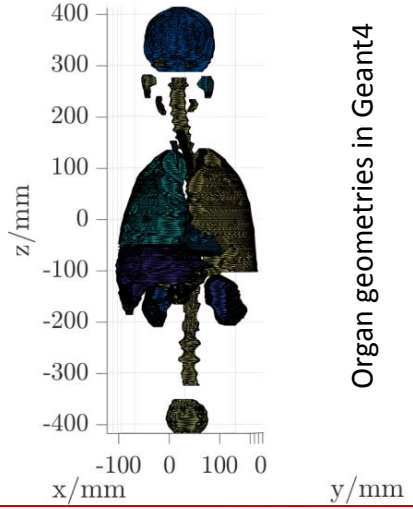


Session 5.3

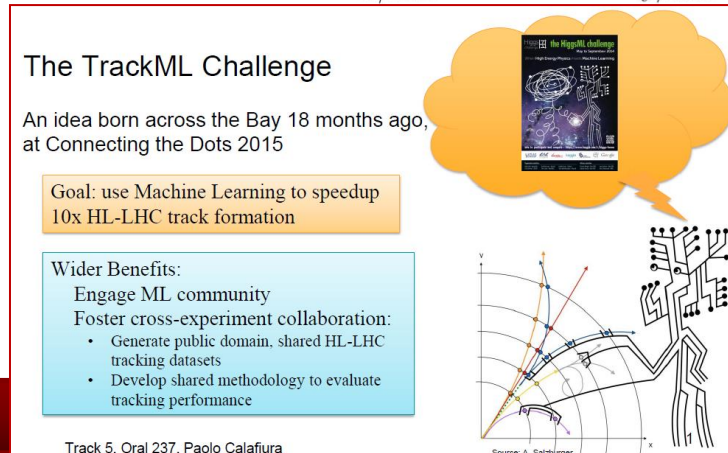
- HEP community is having a deep look at what industry is doing and the tools and the hardware/platforms that are available on a wider scale outside of HEP and in doing so more fields are looking into what we have to offer
  - New possibilities also for outreach, education, and preservation
- The tools we are most familiar with have become more mature all the while trying new ways to improve and interface with the latest technologies
  - Sustainable software development

5.1 Physics Applications and Machine Learning

- **GooFit: a massively-parallel fitting framework** for partial wave analysis on GPUs
- **New simplified event data aiming at FCC, PODIO** supports vectorization, automated code generation, C++ and Python bindings, thread-safe, different I/O layers.
- **Medicine**: dose-toxicity correlations in cancer radiotherapy
  - Online measurement of delivered dose at millimeter-scale volumes and correlate with side-effects
  - **Software framework inspired by Gaudi/Athena**, job management with Ganga and started to work on **GEANT-based simulation** of treatment setup
  - Large processing requirements by cancer research standards
- A.I. techniques can help to solve extremely complex problems
  - First use of **convolutional neural networks** for a HEP result in neutrino appearance analysis at NOvA
  - Raw data feature extraction at Daya Bay with **deep machine learning**
  - **The TrackML Challenge**



Organ geometries in Geant4

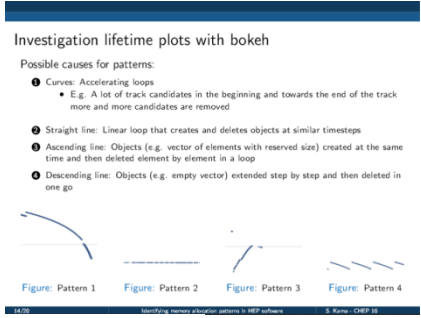


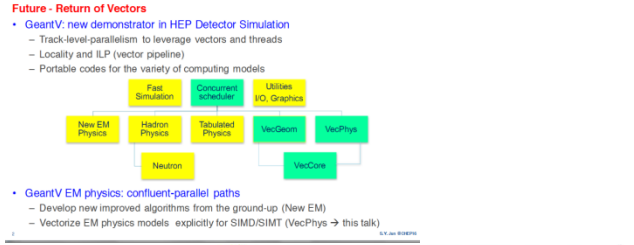
5.2 ROOT EVOLUTION

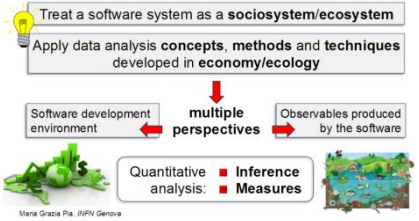
- **ROOT is evolving** along two main directions: development (with a substantial rewriting) of ROOT core and its components and integrating ROOT with other tools and frameworks
- "**doxygen**", i.e. documentation, is the main keyword in commits
- New C++/programming paradigms will improve performance and user experience (e.g. the compilers will be more efficient in detecting errors)
- Gradual transition to new interfaces for **ROOT7**
  - New **ROOT::Experimental** name space for testing and development in closer collaboration with users
- Using **C++ modules** to improve compilation time, in collaboration with Google engineers
  - Preliminary result: **21% compile time reduction**. A lot of old code is being revisited and fixed or improved.
- **Multi-threading/multi-processing support**: parallel processing of branches and entries supported via high-level interface to implicit parallelism
- **Exploring new technologies** like Apache Spark and CERN SWAN service for parallel processing
- **ROOT integration with Jupyter** notebooks: focus on interactivity for machine learning and analysis
  - ROOT tutorial available as notebooks.
- **TMVA** with interfaces to many external toolkits (R, scikit-learn, TensorFlow, ...) and high-performance **GPU integration for Deep Learning**
- node.js integration with ROOT allows access to all **ROOT features from complex web applications**

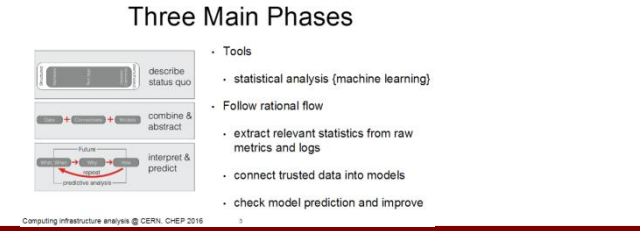
5.3 Performance, Analytics, …

- Even our **largest codes are not unmanageable**: ATLAS performed a multi-months design review of the entire code base
- We can treat our large **code bases as data analytics problem**. There are powerful tools to gather software metrics both statically and at runtime; it helps us to decide where to put coding effort
- New "FOM (Find Obsolete Memory) Tools" is a powerful utility to understand **memory allocation patterns in real-world applications**: they point out a number of seemingly low-hanging fruits such as frequent, short-lived, and small allocations that can probably be avoided
- **Systematic data analytics** of running jobs in data centers can possibly replace synthetic benchmarks (which not necessarily reflect application usage patterns); we should be soon able to somewhat predict job performance from job features.









5.4 Processors, Architectures, …

- **Processors** trends
  - Many-core and vector CPSs, Next generation ARM, PowerPC, Nvidia P100 (after K40)
- …And **applications**
  - Geant4 multithread on MIC
  - Alice processing pipeline on MIC
  - NLO Generators scaling up to top computers

THE NEW ERA: THE CHANGE

The on-chip power density limitations are driving the computing market towards a greater variety of solutions

- ARM announced ARMv8.{0,1,2} which covers server market
  - Designs with up to 64 cores announced & to be used in supercomputers
- ARM recently announced Scalable Vector Extension (SVE) for HPC
  - Up to 2K vector sizes & binary compatibility
- IBM announced OpenPOWER Foundation which allows other companies to build PowerPC CPUs
- POWER9 (based on PowerISA 3.0) is the first one after OpenPOWER Foundation was launched
- IBM recently announced POWER8+ with NVLink 1.0 support
- Intel recently announced KNL (many-core and vector CPU) with legacy support for x86_64

http://www.geant4.org

Multi-threaded Geant4 on Intel Many Integrated Core architectures

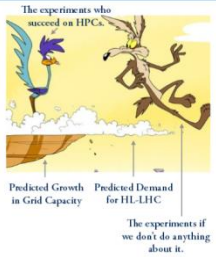
Starting from Geant4 Version 10.x : focus on parallelism
- Multi-threading: **memory reduction** (factor 10 w.r.t. multi-process) achieved
- Lock free event loop: **almost perfect scalability** (>90% linearity) with large number of threads
- Hybrid MPI/MT jobs: **achieved on very large number of workers** (256k total threads)
  - Test jobs on hybrid host/KNC shows good results

KNC supported since few years, preliminary tests on KNL confirm scaling and memory redcution
- **Factor 3 speedup w.r.t. KNC achieved**
- Simplified workflow and access to large DDR3 memory: more complex jobs possible

Started testing on SuperComputers with massive parallelism (MIRA@ANL):
- With more than ~100k workers I/O is limiting scaling (not specific to G4): plans to mitigate effect are in place
- Next generation of SuperCompouters based on KNL: Theta@ANL, CoriII@NERSC
  - Getting ready to run complex simulations!

Motivation

- As we have seen in many talks at CHEP, LHC computing needs are expected to grow by more than a factor of 60 through the HL-LHC.
- Any cpu cycle offloaded to an HPC frees up a cycle on the Grid.
- NLO generators, like Sherpa & MadGraph5_aMC@NLO, involve computationally intensive integrations.
  - In Sherpa, W+4 jets with 1% precision requires a 16-core Intel Xeon 6.5days to compute.
- Increased multiplicity and going to NNLO will continue to increase the compute time of these calculations.
- Scaling codes on leadership machines reduces the time to get results and these optimizations typically result in better efficiency on all systems.



CHEP San Francisco J. Taylor Childers October 2016

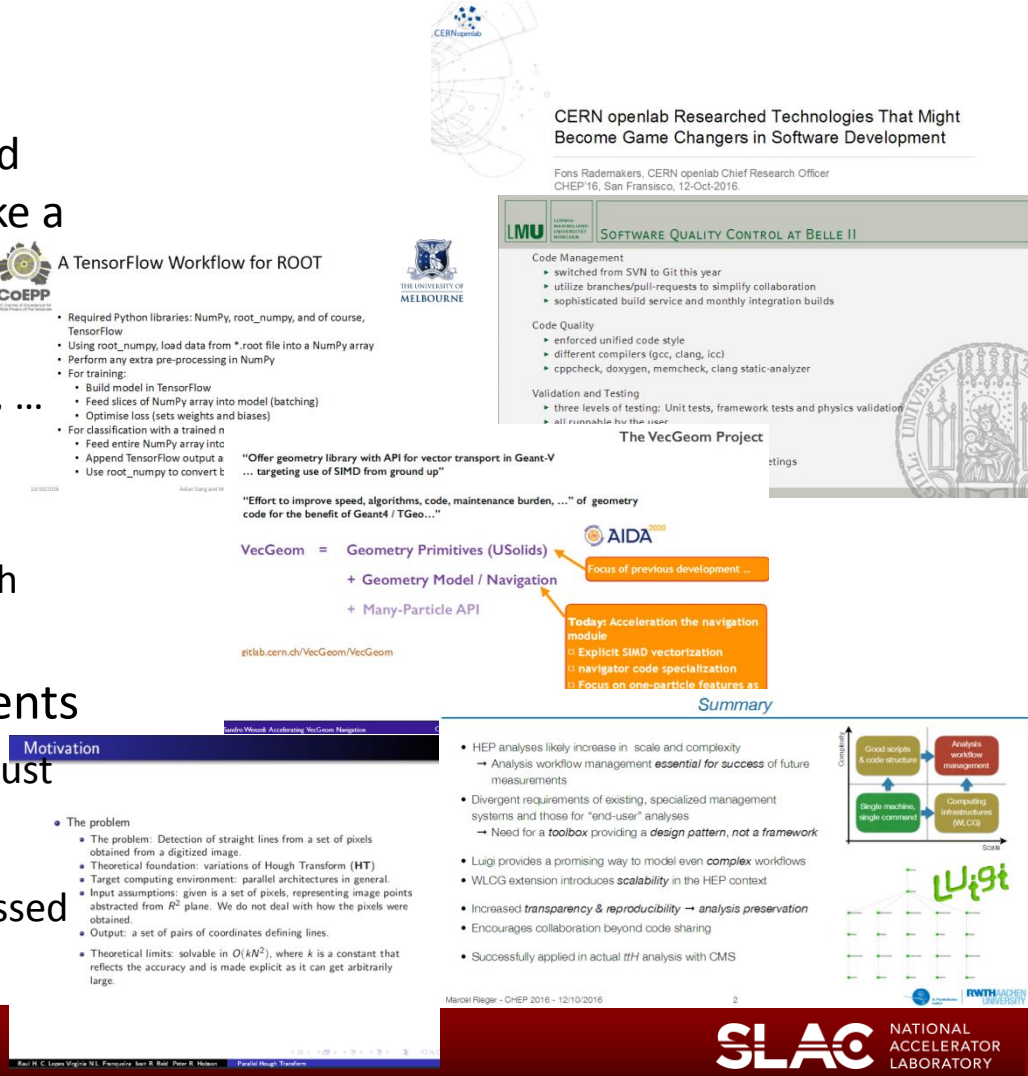
What's a Xeon Phi ?

- Device from Intel
  - Intel Many Integrated Cores (MIC)
  - KNC (2013), KNL (2016)
- Form factor
  - (big) PCI-E "co-processor" (KNC, KNL soon?)
  - Standalone systems, integrated fabric (KNL)
- Specifications highlights
  - 57-72 physical cores
  - x86 cores, based on Pentium (KNC) / Atom (KNL)
  - 4-way multithreading
  - Moderate core clocking (1.1-1.5 GHz)
  - Large vectors (512b)
  - Fast on-chip MCDRAM (KNL, 8-16GB)
  - Power 200-300 W
- Potentially interesting for some processing tasks

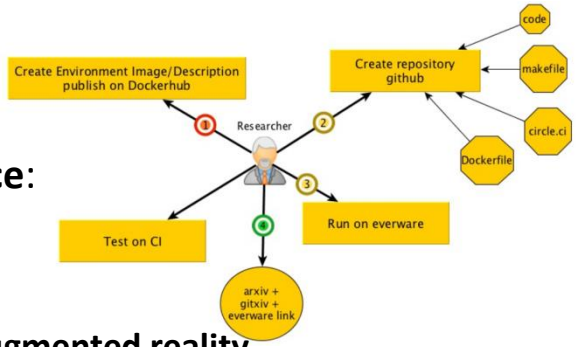
> cat /proc/cpuinfo | grep processor | wc
256

5.5 Software

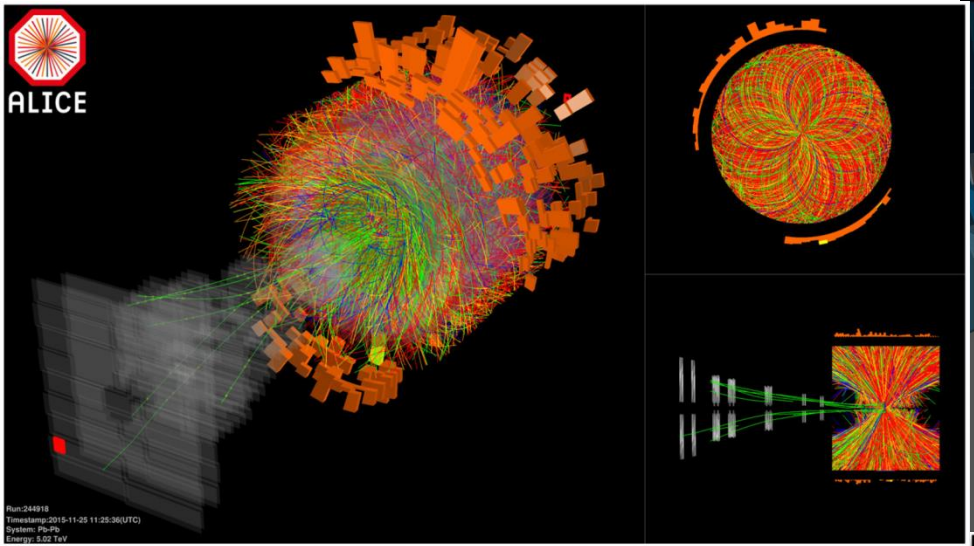
- Software and algorithm **optimization**, and modern technologies together could make a difference
  - 3D Xpoint NVRAM, XeonPhi, NVidia, …
  - Structure of Arrays to Array of Structures, …
  - Vectorization
  - Machine learning with TensorFlow
  - New algorithms (track reconstruction with Hough transform)
- New **computing models** for experiments
  - Modern code management, efficient, robust
- New analysis **workflows**
  - Scalability and complexity must be addressed with new set of tools

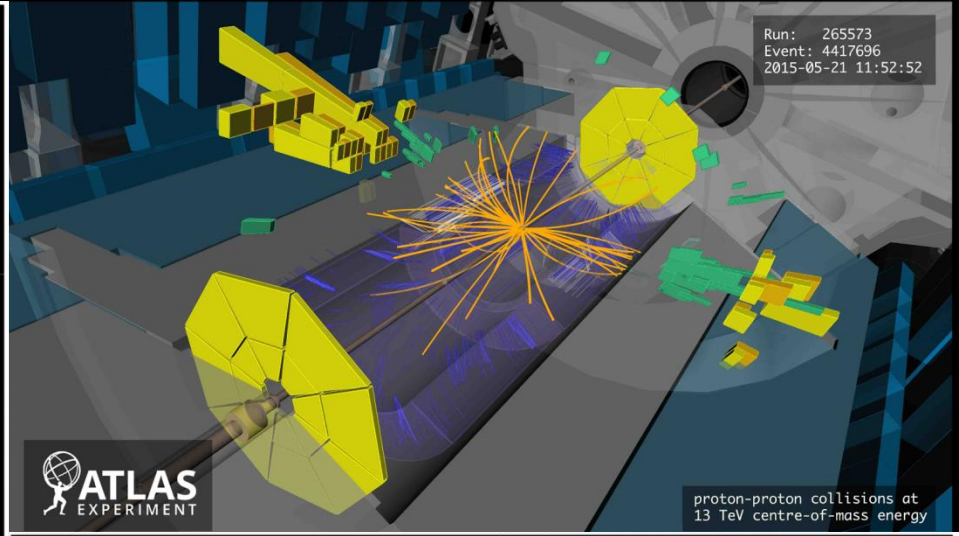


5.6 VISUALIZATION

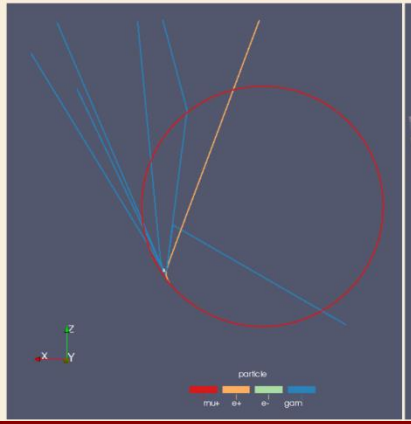


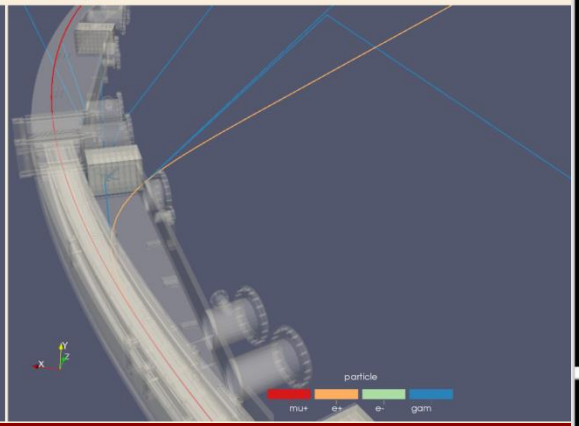
- Clear trends toward using **less "in-house solutions" and use best practice**:
  - WebGL and web standards, jupyter / python, Paraview
- Experiments **event display**
  - ALICE: based on AliEVE, very attractive possibilities for outreach, including **augmented reality**
  - Belle II: **jupyter** based notebooks **for full analysis in your browser** (experiment agnostic tools developed)
  - ATLAS: Two separate solutions, ATLANTIS and VP1. VP1-light under development for **standalone "laptop" visualization (and outreach)**
  - CMS: WebGL event display based on web-technologies. Independent of CMSSW allowing usage in **education** context (even w/ limited resources)
- **Experiment agnostic tools**
  - Paraview: being developed for g-2 a scientific application with advanced capabilities (client scriptable via **python/numpy**), client-server (catalyst) data processing framework (art) pushing objects for visualization
  - Everware: addressing problem of **reproducibility of scientific results**. Use best practice to increase open access by publishing full analysis "containerized" systems

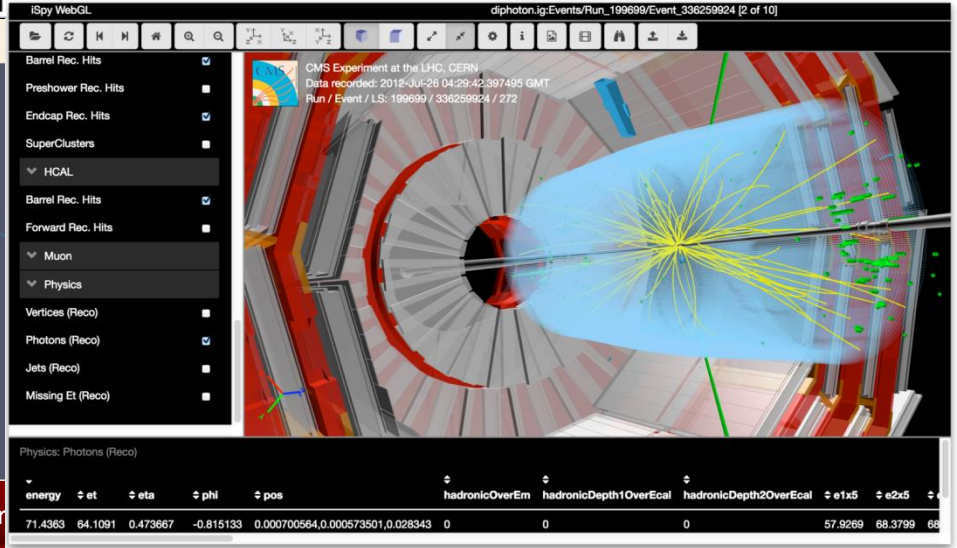




Example, Muon g-2 Geant4 Steps

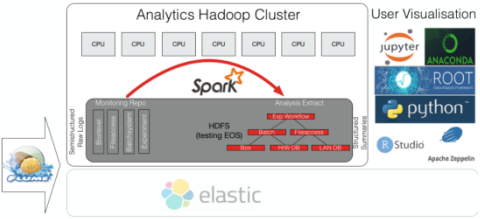


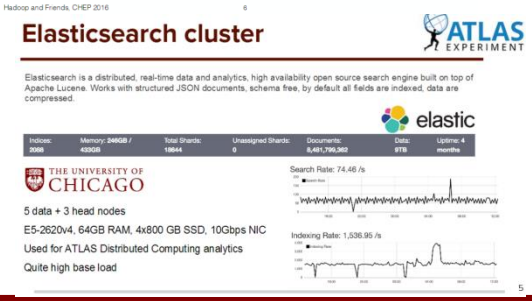


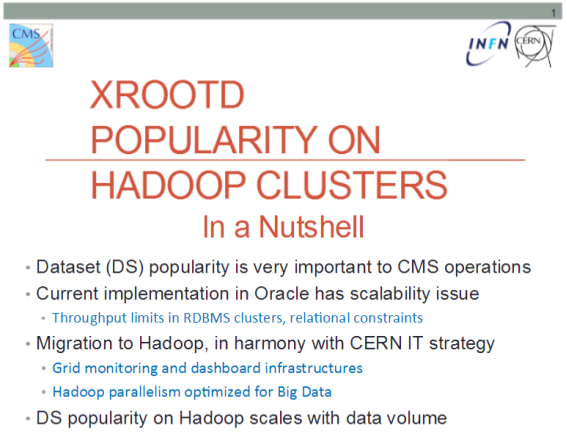


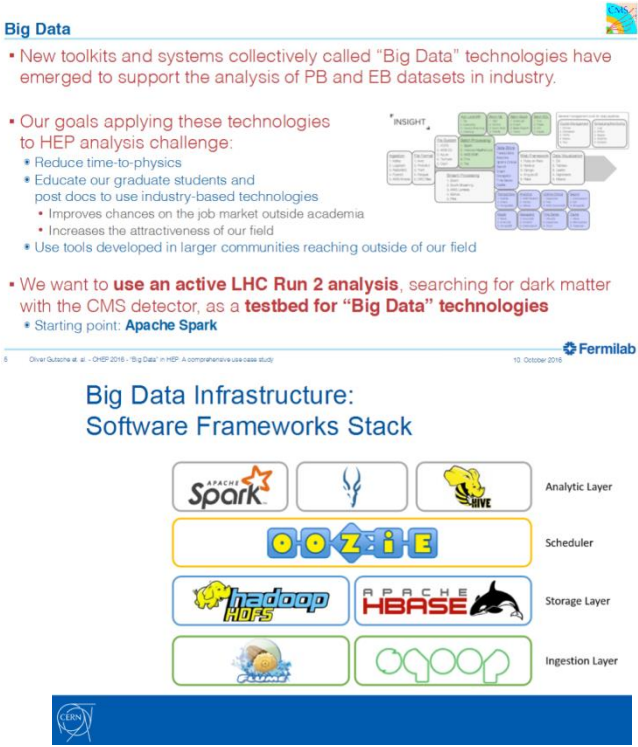
5.7 Big Data

- Big data tools available in **industry** come in focus for physics analysis
- Studies for example on usability of **data storage** in Hadoop, Elasticsearch for indexing of events, and Spark/Scala applications









THANK YOU!

- Thank you to all the speakers, poster presenters, session chairs, session helpers, program committee, and to the conference organizers!