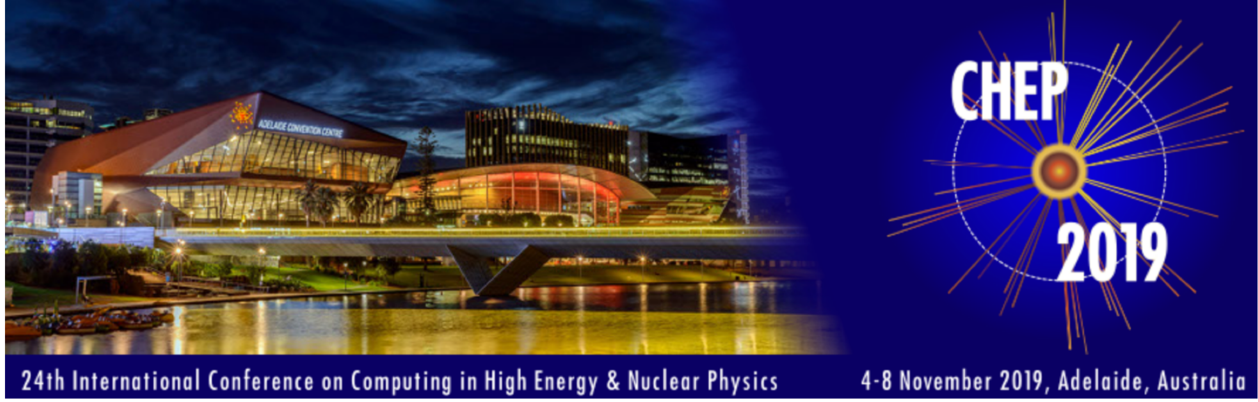


Evolving Geant4 to cope with the new HEP computing challenges

A Gheata for the Geant4 Collaboration

4-8 Nov 2019, Adelaide

Context

- Increasing requirements for simulated samples towards HL-LHC
  - Full simulation still a bottleneck in many workflows
  - Speedup of several factors needed
- Potential of speedup in Geant4 on CPUs now better understood
  - Results from previous performance R&D studies
    - International R&D effort producing GeantV prototype and VecGeom
  - Restructuring and optimizations: more compact and streamlined code
  - Vectorizing some FP-intensive modules (e.g. field integration, multiple scattering)
- Accelerators and heterogenous computing become even more important
  - Making simulation code accelerator friendly becomes a necessity
  - Integration in experiment-driven parallel frameworks essential

Geant4 Task Force for R&Ds

- Created to promote & survey R&D on software architectural revisions
  - Including adaptations to emerging technologies and architectures beneficial to Geant4
- Provide communication/support among/for R&D activities
- Assess performance of different improvements and effort for integration
  - Make recommendations to the Geant4 SB
- Intended as catalyzer for short-cycle integration of performance developments
  - Coming from within and outside the collaboration
  - Regular meetings focused on ideas & follow-up of R&D activities

Performance: main directions

GEANT4
A SIMULATION TOOLKIT

Parallelism

Concurrency model review - fine grain parallelism

Optimization

Faster physics/geometry algorithms - low level code optimizations

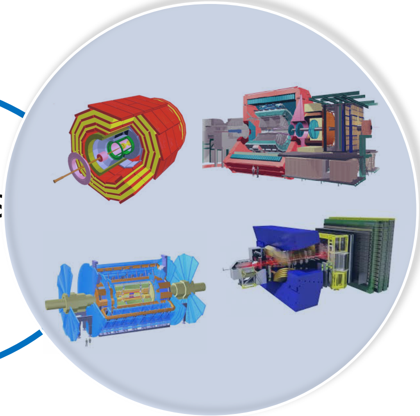
Restructuring

More compact code & data - simplified calling sequence - stateless - pipelines for heavy computation kernels

Heterogenous computing

GPU friendly kernels

Experiments integration



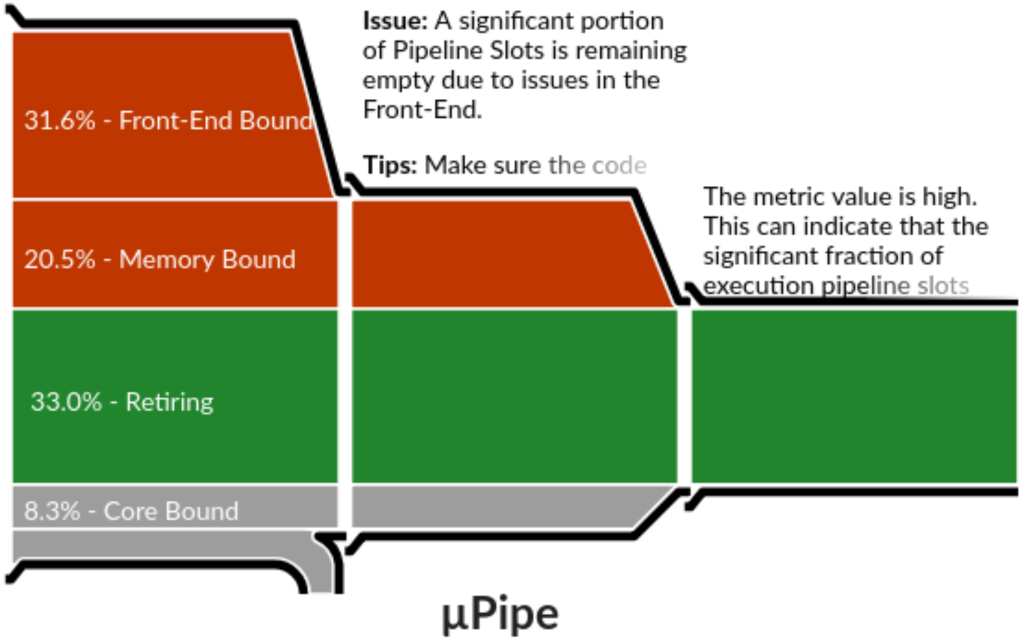
Fast sim revisiting

Parameterizations - ML

Ongoing Investigations

- Code compactness, simplified calling sequence, optimizations
  - A large part of the GeantV speed-up coming from better fitting the instruction cache
  - More streamlined computation for HEP simulation hotspots
- More flexible parallelism model, accelerator friendly
  - Sub-event parallelism, task parallelism
  - Efficient track-level parallelism on warps
- Standardized and easy to use tools enabling fast simulation workflows
  - Parameterizations, but also generative models

Example of CPU µ-pipe for CMS EM shower simulation w/ Geant4

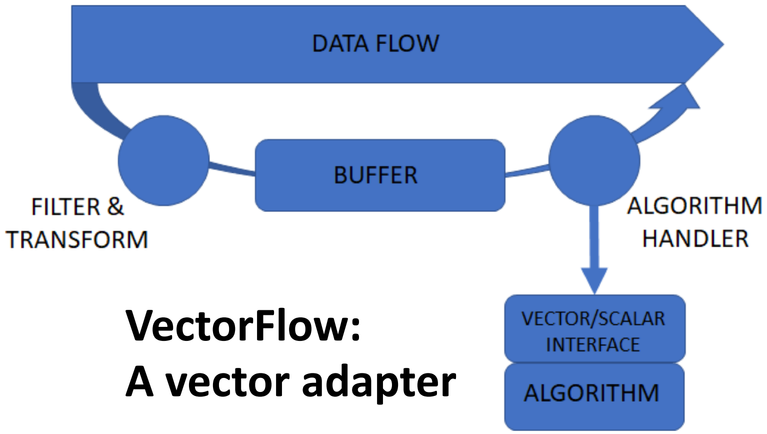


Vtune Microarchitecture analysis
Xeon®CPU E5-2630 v3@2.4 GHz

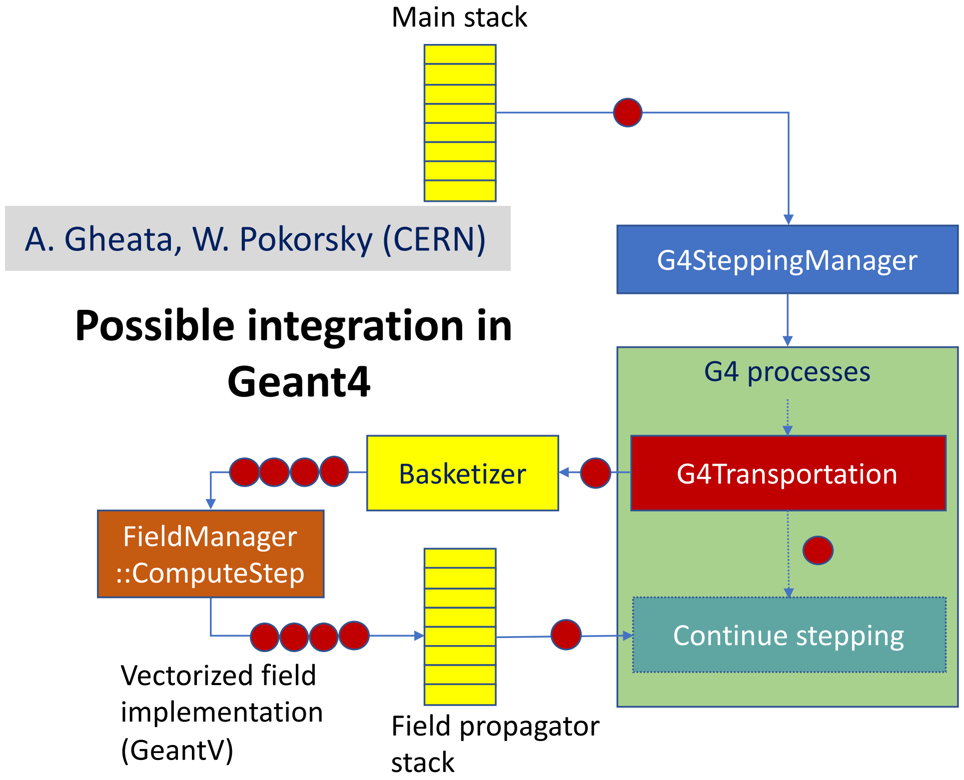
Vector pipelines in Geant4

Generalizing vectorization by passing vectors of data to functions rather than rely on inner loops.

- Idea originating from GeantV workflow, but generalized as templated API usable in any workflow
  - Using VecCore as vectorization library
- Prototyping the changes needed in Geant4 for such extension
  - Ongoing work for making Geant4 transport stateless
  - Aiming to prototype integration w/ FP-intensive modules



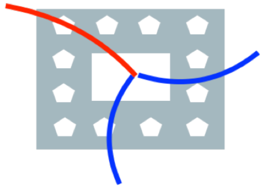
VectorFlow: A vector adapter



Possible integration in Geant4

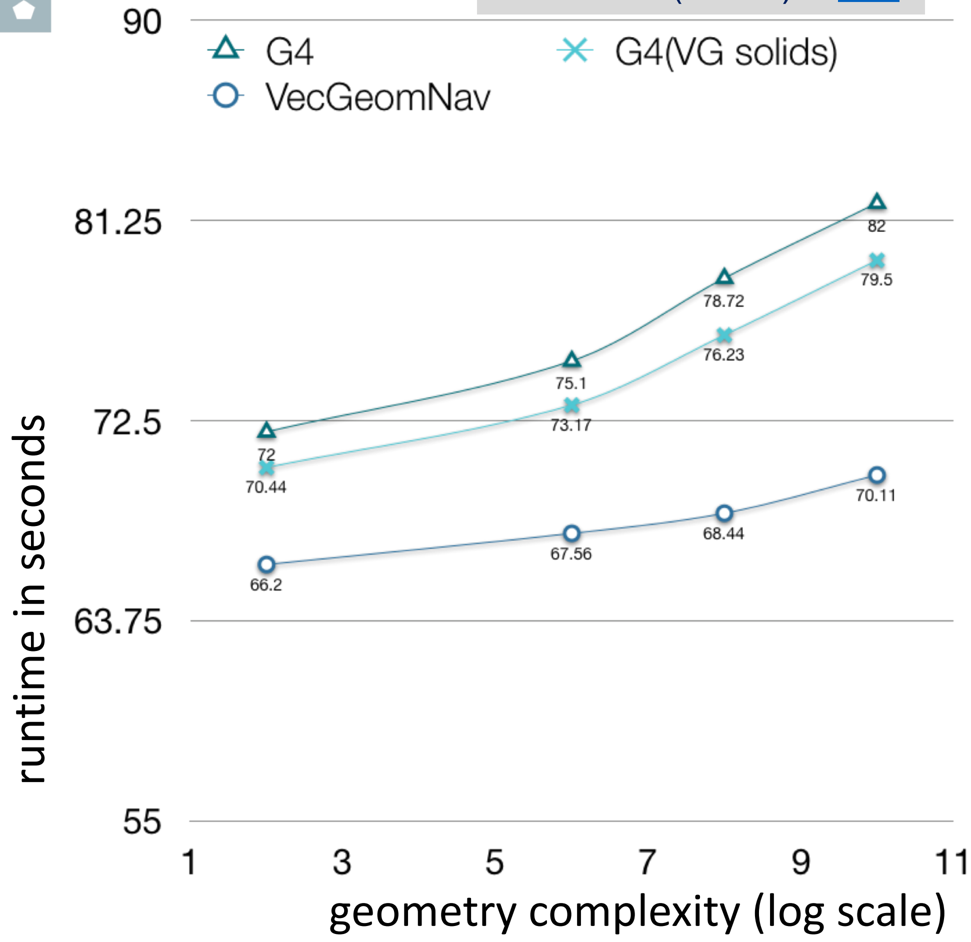
Optimizing Geant4 navigation using VecGeom

VecGeom



- A first implementation of a Geant4 **navigation plugin**, using VecGeom capabilities.
  - Allows to make use of the modular and extensible navigation acceleration structures of VecGeom
- Tests on full detector geometries remain to be done and development to be completed
  - Preliminary tests on simplified geometry very promising: 10-15% speedup vs. G4 native geom
- Related ongoing work: VecGeom navigation specialization for some volume topologies

S. Wenzel (CERN) - talk



Parallelism model, GPU exploration

Extension of Geant4 parallelism model to a task approach

GPU exploration work in general HEP simulation context

Task parallelism in Geant4

J. Madsen (LBL)

- Geant4 can benefit from having internally nested task-based parallelism
  - Making parallelism transparent to users (i.e no G4MTRunManager)
  - Better support for sub-event parallelism, eventually track-level parallelism
- Easier to expose simulation as a task
  - In relation with concurrent task based frameworks (e.g. CMSSW, Gaudi, …)
- First implementation of tasking support already available
  - gitlab.cern.ch/jmadsen/geant4-tasking
  - Based on standalone tasking library: github.com/jrmadsen/PTL
    - Native C++ features (future, promise, packaged_task, coroutines)
    - TBB backend available, PTL forwards task to TBB scheduler instead of internal
  - Support for multiple task pools
    - E.g for off-loading work to coprocessors

Exploring GPU usage in full HEP simulation

P. Canal (FNAL), J. Madsen (LBL) et al talk

- Geant Exascale Pilot Project – several collaborators from US
  - Goal to **study and characterize architecture and performance** to best use GPUs in general and Exascale facility in particular for full HEP simulation
    - Explore memory access, computation ordering, and CPU/GPU communication patterns
    - Avoid over-simplification
    - Reuse or leverage existing packages, not bound by backward compatibility
  - Strategies
    - Focus on NVidia compiler at first (later look at Kokkos and others)
    - Research way to increase instruction and data cache efficiency
  - Early technical ideas
    - **Partial Static Polymorphism**: allow upload/download of data to device without transformation
    - **Separation Of State and Access and Functional Approach**: allow significant data memory layout change without code change

- GPU-aware physics code restructuring being investigated
  - Kernels for EM shower physics “confined” to GPU, w/o user code calls

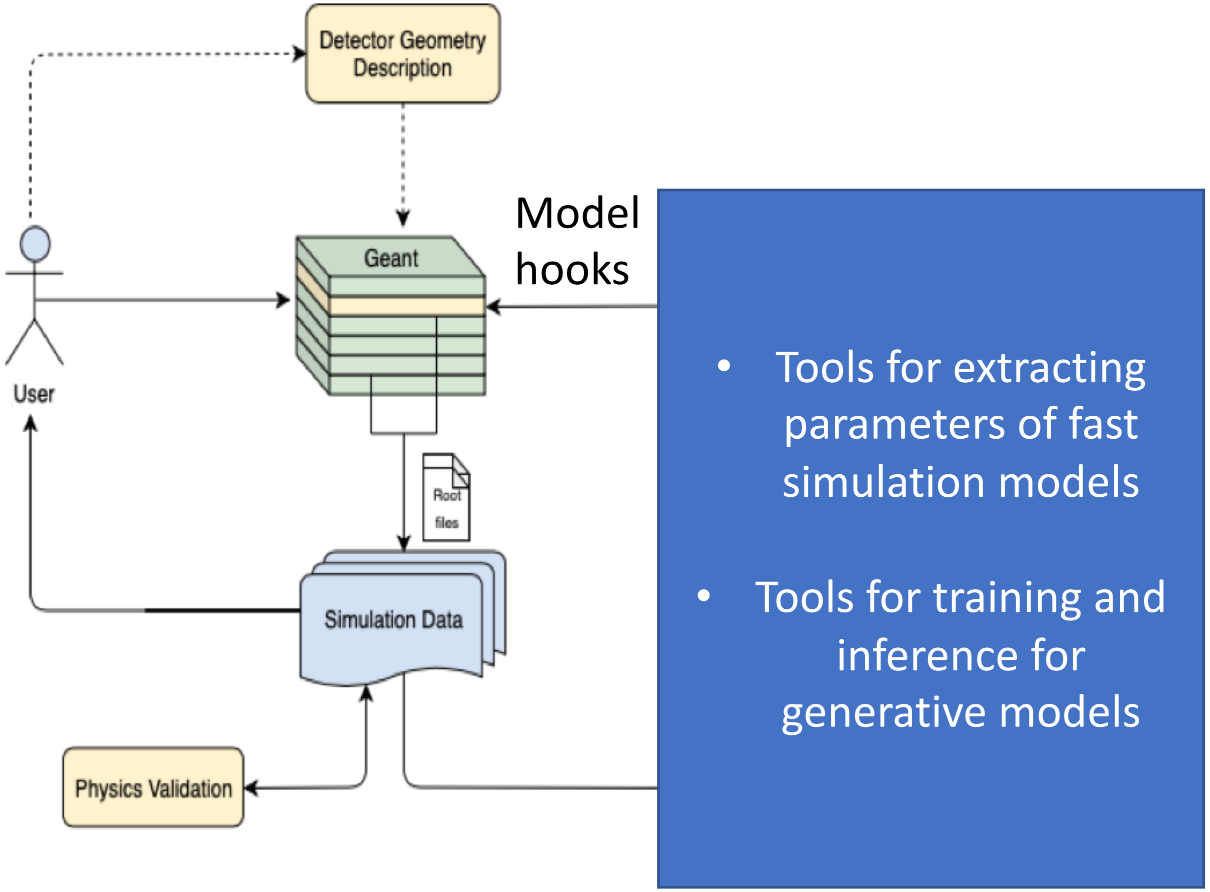
Fast simulation toolchains

fast simulation techniques use approximations which typically trade accuracy by speed (e.g. shower libraries, parameterizations, sampling, ML)

Integration with Geant4-based full simulation workflows can be standardized

Automated tools for fast simulation

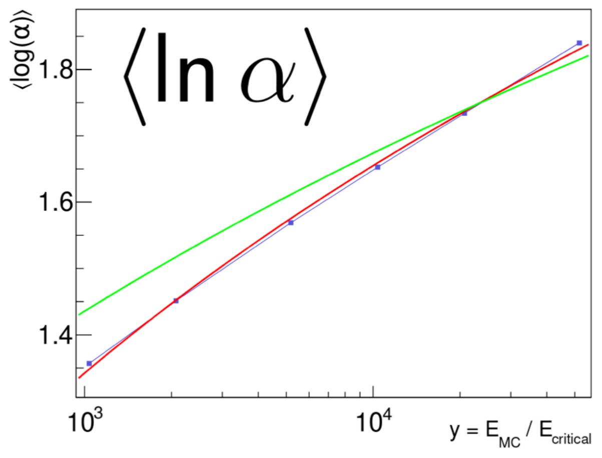
- Fast simulation is experiment dependent
  - custom procedures to extract parameterisations
- Ongoing work for streamlining the procedure
  - ➢ Users come with their own setup
  - ➢ Full simulation producing standard information (hits)
  - ➢ Simplified, automatic and easy to use procedures to extract the parameters (e.g. fitting shower profiles, training networks)
  - ➢ Plugged back in simulation via Geant4 fast sim hooks
- Goal: improve precision of fast simulation models

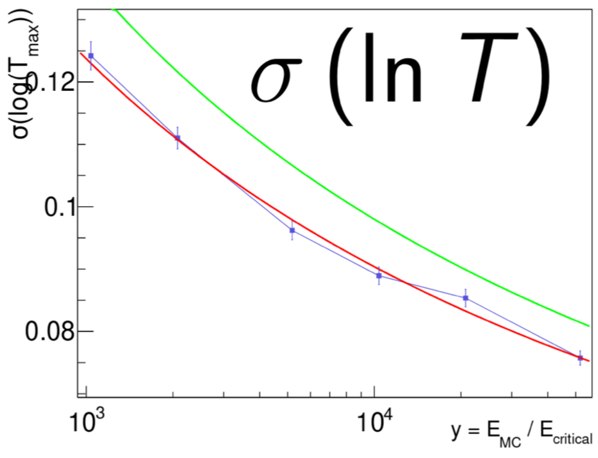


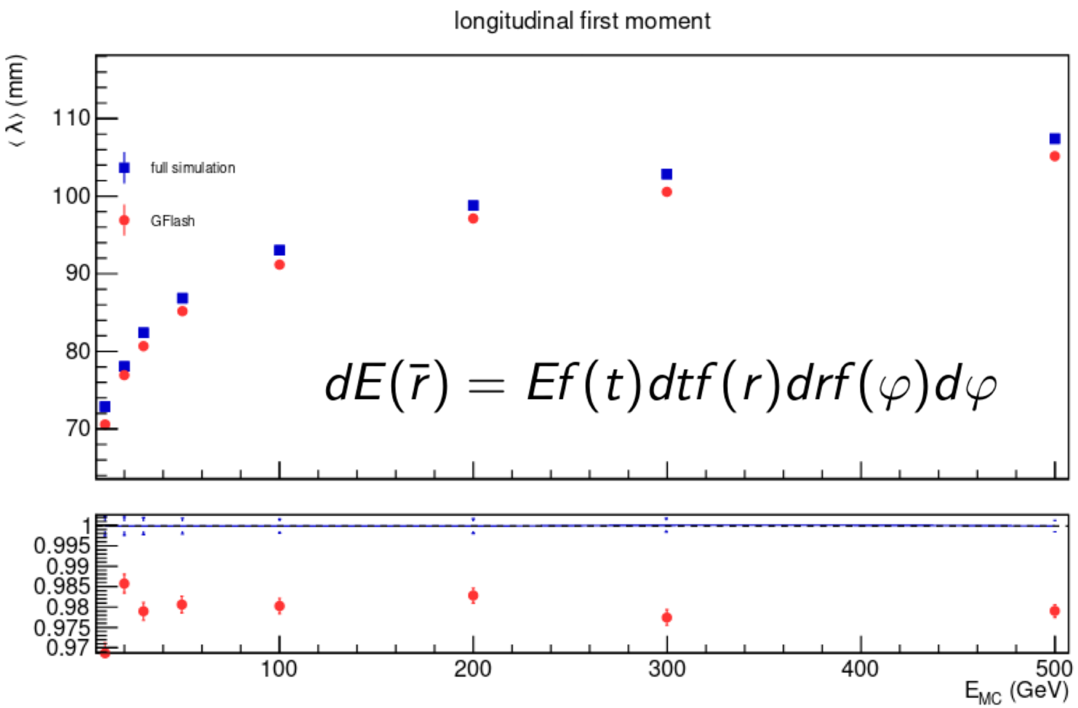
Automating parameterisation for fast simulation

- Revisiting fast simulation hooks and models offered by Geant4 (e.g. GFlash).
- Work on automation of EM shower parametrisation - tuning of parameters for users' geometry.
- More validation tools developed (for fast simulation, biasing - comparison to standard simulation)

A. Zaborowska (CERN)



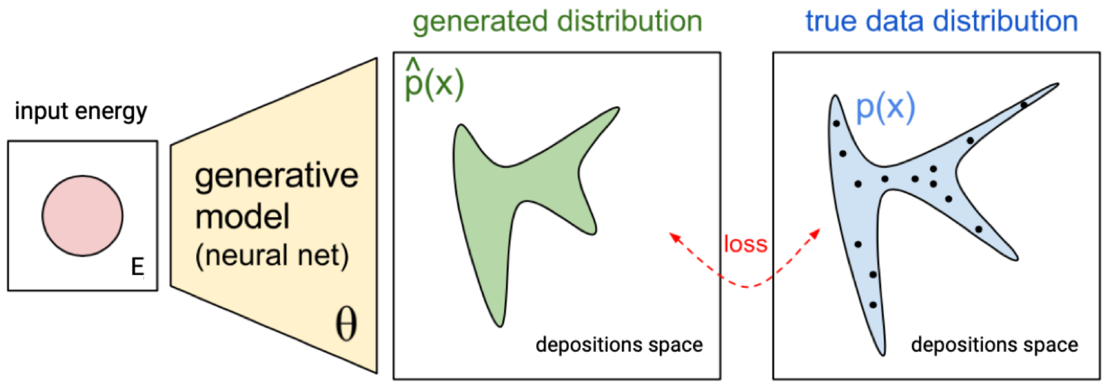




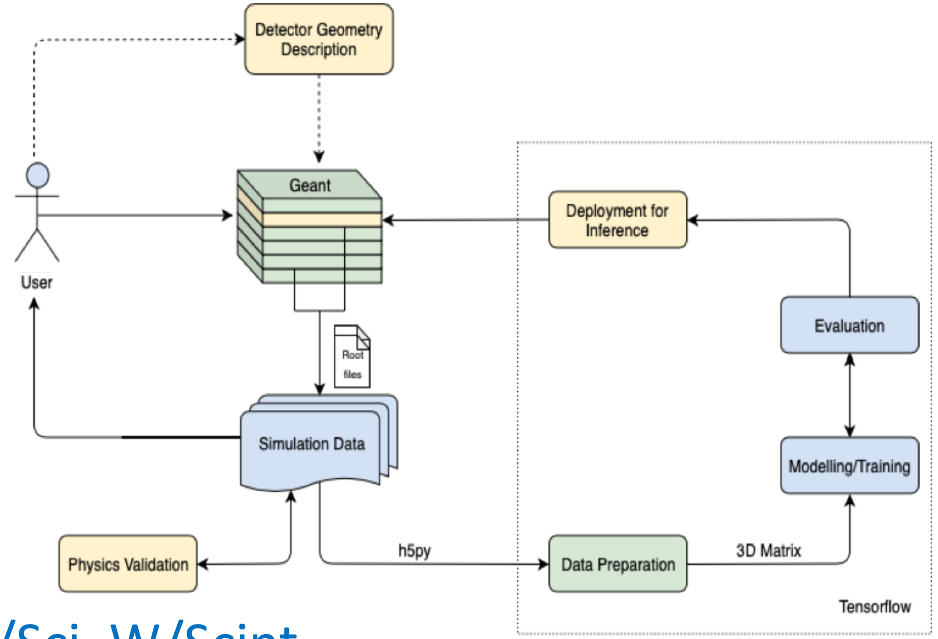
green line - GFlash parameters from arXiv:hep-ex/0001020
blue points - from full simulation on Pb
red line - fit to full simulation (e.g. no Z dependency)

Machine Learning Approaches

I. Ifrim (CERN) talk and poster



https://openai.com/blog/generative-models/



- Training on simulated data
  - Different calorimeter types : PbWO4, Pb/LAr, Pb/Sci, W/Scint
- Different architectures are tested
  - Autoregressive, VAE, GAN
  - Validation against MC truth
- Training/inference workflow aiming to integrate with Geant4 hooks
  - R&D done in EP-SFT & openlab (CERN)

Other optimizations and new features

- Magnetic field class refactoring
  - Runtime -> static polymorphism
  - Multi-particle driver integration
- Sub-event parallelism
  - Allow splitting events in vertices processed by separate threads
  - Better scaling and MT workload for large events
- Refactoring transportation
  - Splitting transportation process in “flavors” dealing separately with:
    - Charged/neutral particles, optical photons, parallel geometries or other specialized cases
  - Increasing code locality and decreasing branching

Conclusions

- Geant4 puts very high priority on performance related developments
    - Task force for R&D as catalyzer for development & integration
- Several performance improvement directions being followed
    - Structural changes & optimizations, but also revisiting fast sim workflows
- R&D on extending the parallelism model
    - More efficient integration with experiments parallel frameworks
    - Targeting also accelerators and HTC
- Aiming for accelerated prototyping/integration cycle