Detector Simulation

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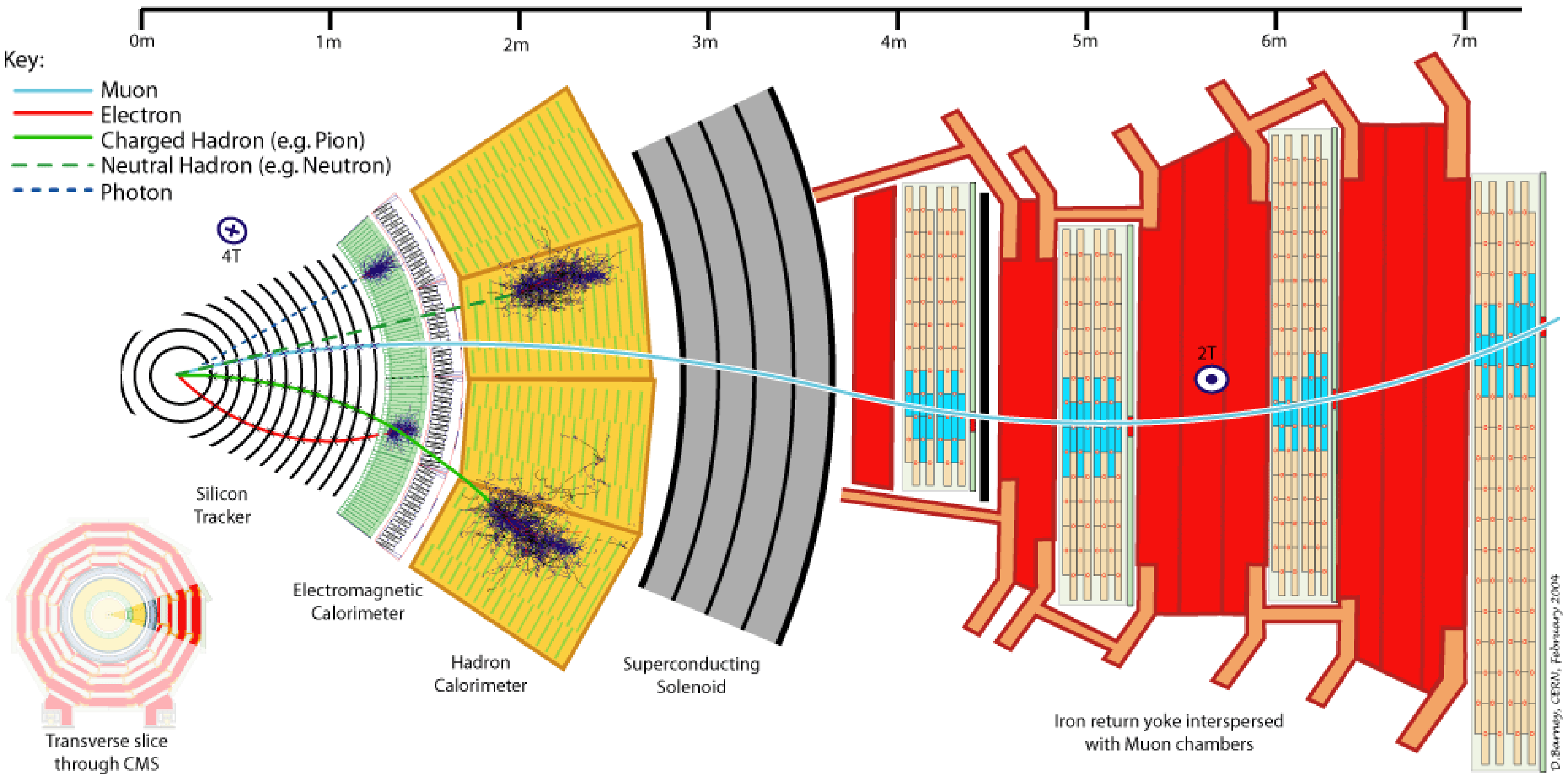
Personal Intro

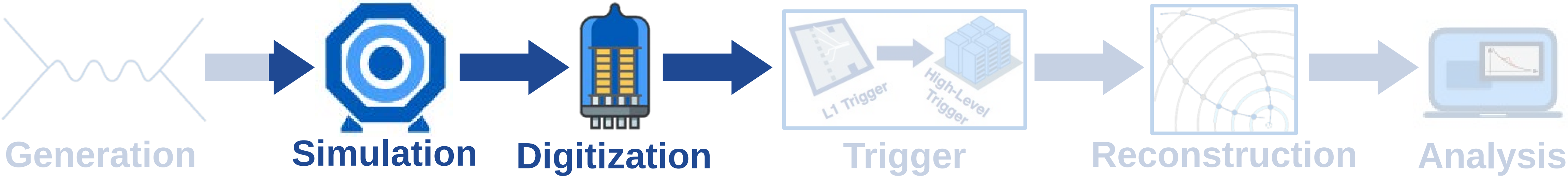
- Who am I?
  - Associate Scientist in Fermilab’s Computational Science and Artificial Intelligence Directorate
  - Incoming CMS Simulation Convener, and formerly:
    - CMS Upgrade Software Coordinator
    - HEP Software Foundation Simulation Working Group Convener
    - Snowmass Computational Frontier Theoretical Calculations and Simulation Convener
  - Technical research in software, computing, AI/ML
  - Physics interests: strongly coupled dark matter (“dark QCD”), supersymmetry
- How did I get involved in simulation?
  - As a graduate student, interested in simulating new calorimeter designs for CMS detector upgrades
    - An interest many of you may soon share, as future collider programs start ramping up!
  - Simulation underpins everything else that we do in HEP
    - But nevertheless an underserved area – good place to make an impact!

What Happens at Colliders



- Our question today: how do we come up with an *expectation* for what will happen?
  - Critical for design, calibration, analysis, etc.
- Side note: ~2/3 of hadrons (at typical energies) actually start to shower in the ECAL

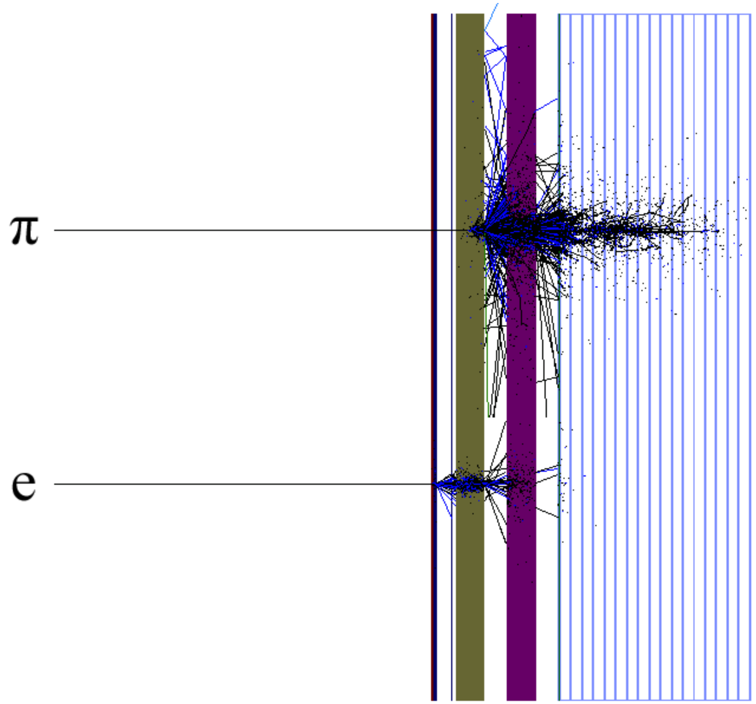
Monte Carlo Production Chain



- Observed outcomes of quantum processes appear random
- We use Monte Carlo simulation to make statistical predictions
  - Randomly produce many events, sampling from expected distributions
  - Simulate every step between initial proton-proton collision (hard scattering) and reconstruction of high-level objects and variables
- This lecture focuses on detector (and electronics) simulation
  - Other steps addressed by other lectures at the school

Full Detector Simulation

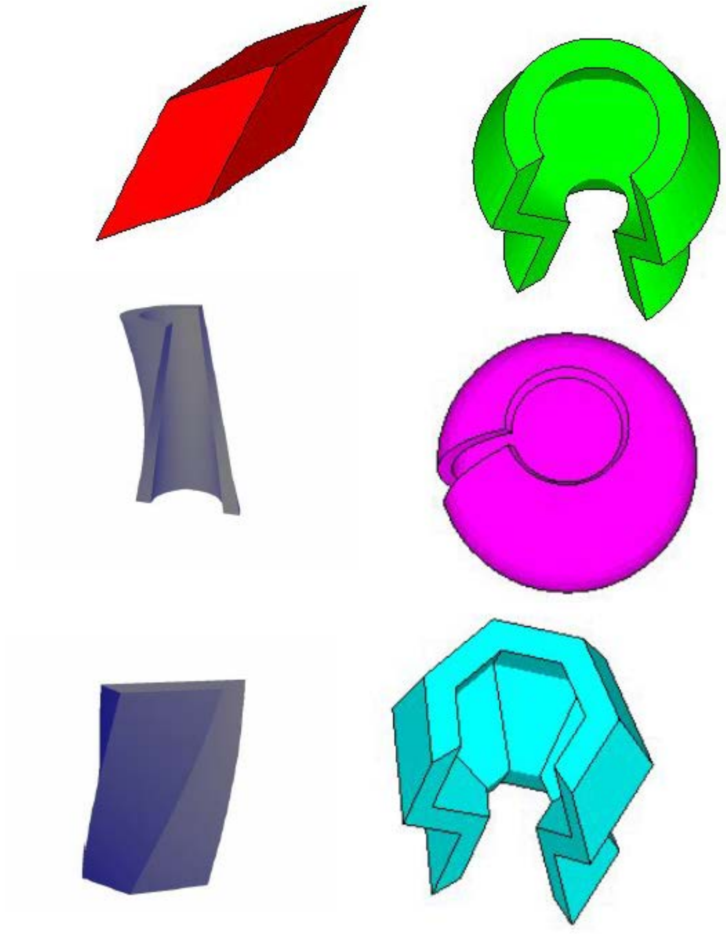
- GEANT: GEometry ANd Tracking
- Geant4: first released in 1998, now on 11th major version
  - C++ software with multithreading support
  - Successor to Geant3 (1982, Fortran)
  - Developed by international collaboration
  - Used for more than just HEP:
    - Space, medicine, microelectronics, nuclear physics
      - Essentially anywhere radiation modeling is important
- What does full detector simulation entail?
  - Modeling of: geometry, materials, particle trajectories, interactions, decays, detector responses
    - Not all decays handled by generators (e.g. hadrons)
    - Charged BSM particles need to be implemented manually



A visualization of pion and electron showers in a CMS-like calorimeter (from my aforementioned graduate work)

Geometry

- Detectors are composed of many pieces
  - Some have regular shapes (solids, polyhedral)
  - Others have more complex shapes
    - Defined by additional parameters, e.g. twisted solids
  - Even more complex shapes can be defined by composing, subtracting, etc. simpler shapes
- When constructing an entire detector, repeated shapes can be cloned and automatically assigned unique numbering
  - Helpful for sampling calorimeters like CMS HCAL
- Geant4 has built-in geometry tools
  - More sophisticated geometry management available from DD4hep software
  - Both can use GDML (Geometry Description Markup Language, based on XML)



Materials

- Predefined materials with measured properties from NIST Physical Reference Data
  - Another good reference: PDG Atomic and Nuclear Properties of Materials
- Multiple ways to create new materials:
  - Start from existing material & modify properties
  - Assemble from elements into molecules, mixtures
- Correct modeling of these properties is essential to understand how particles interact with detector materials
  - Automatically computed properties for new materials usually fairly accurate, but measurements are best

Atomic and nuclear properties of polystyrene [$(C_6H_5CHCH_2)_n$]

Quantity	Value	Units	Value	Units
<Z/A>	0.53768	mol g^{-1}		
Density	1.060	g cm^{-3}		
Mean excitation energy	68.7	eV		
Minimum ionization	1.936	MeV g^{-1}cm^2	2.052	MeV cm^{-1}
Nuclear interaction length	81.7	g cm^{-2}	77.07	cm
Nuclear collision length	57.5	g cm^{-2}	54.24	cm
Pion interaction length	113.9	g cm^{-2}	107.5	cm
Pion collision length	85.0	g cm^{-2}	80.16	cm
Radiation length	43.79	g cm^{-2}	41.31	cm
Critical energy	93.11	MeV (for e^-)	90.65	MeV (for e^+)
Muon critical energy	1183.	GeV		
Molière radius	9.97	g cm^{-2}	9.409	cm
Plasma energy $\hbar\omega_p$	21.75	eV		
Index of refraction (Na D)	1.590			

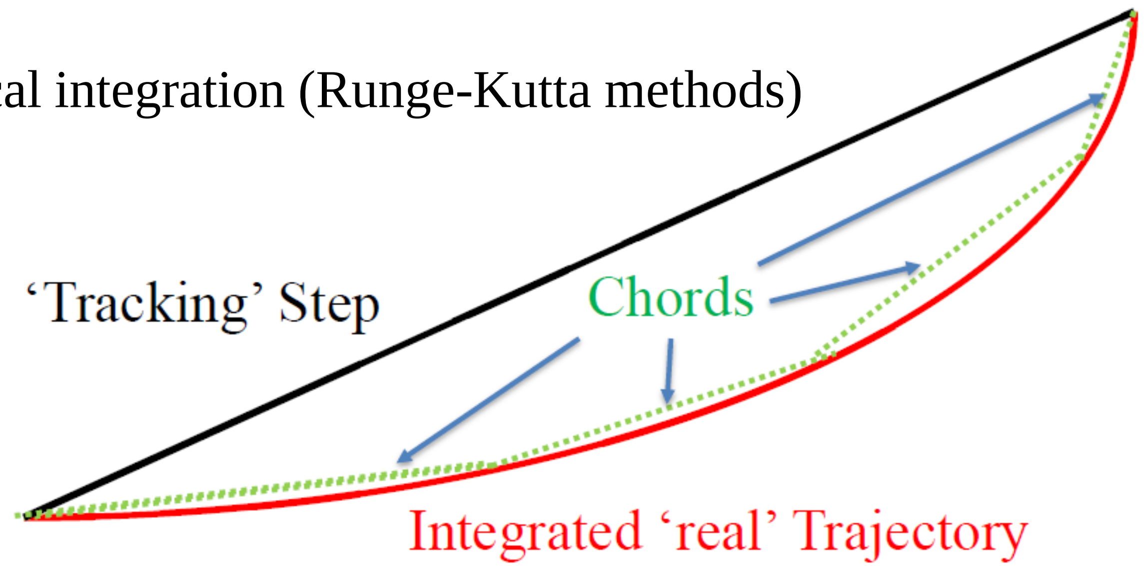
Composition:

Elem	Z	Atomic frac*	A	Mass frac
H	1	8.00	1.0080	0.077418
C	6	8.00	12.0107	0.922582
* calculated from mass fraction data				

For muons, $dE/dx = a(E) + b(E)\ E$. Tables of $b(E)$: PDF TEXT
Table of muon dE/dx and Range: PDF TEXT
Explanation of some entries

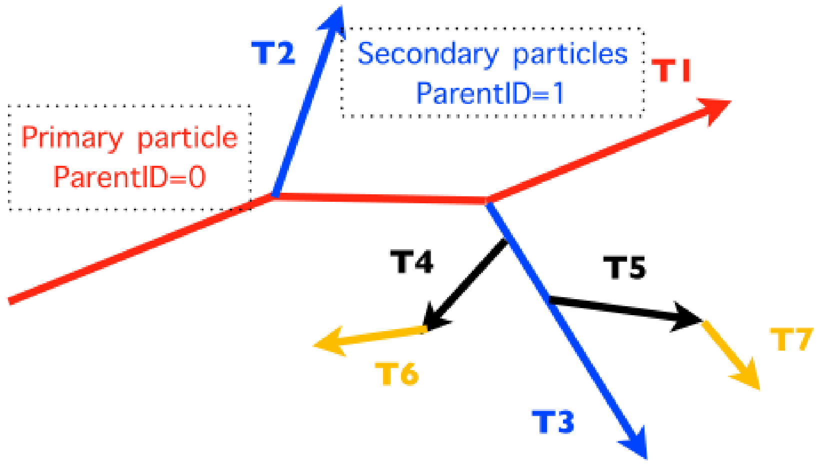
Tracking

- Let's assume we've completed two steps so far:
  1. Generated collision events → list of final-state particles (ID, position, momentum, charge, etc.)
     - GEANT4 has built-in particle guns for simple cases
  2. Built a representation of our detector: geometry and materials
- Next step: propagate particles through the detector → *tracking*
  - Create a series of copies of each particle as it traverses the detector and its properties change
- Important aspect: magnetic fields
  - Specify properties of the field (usually not uniform)
  - Solve equation of motion to find trajectory: numerical integration (Runge-Kutta methods)



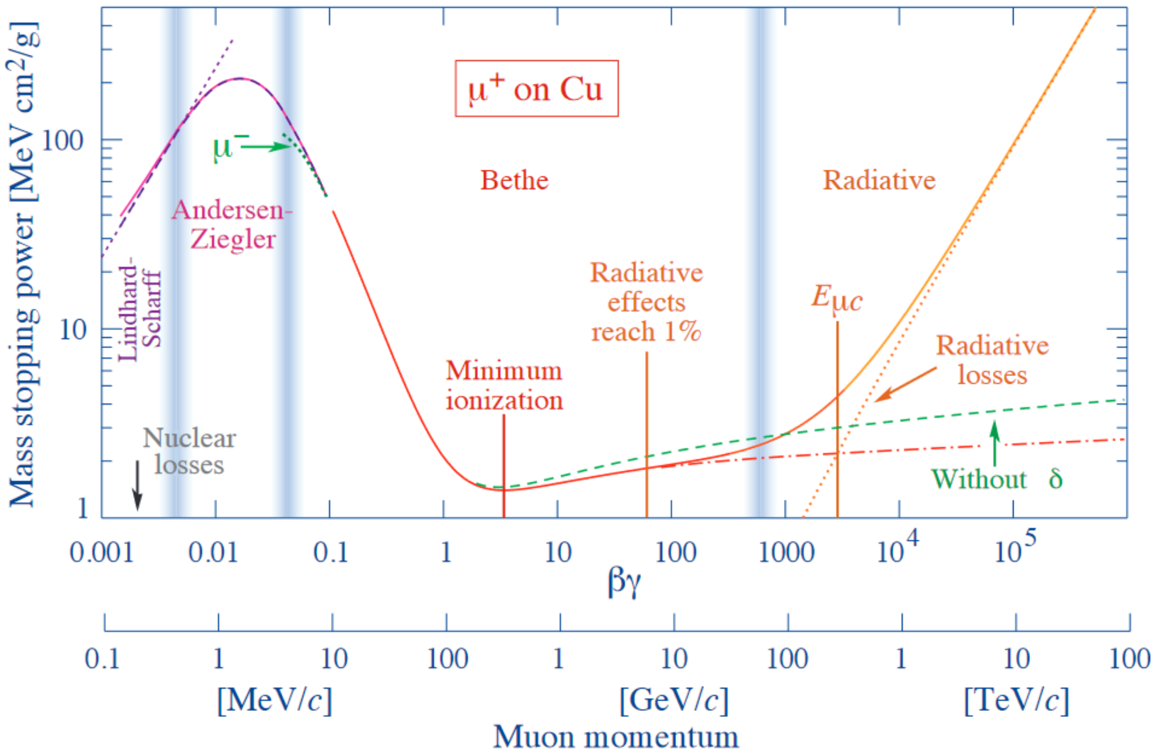
Interactions

- As particles traverse the detector, they *interact* with the detector materials
  - o Through these interactions, particles lose energy and produce secondary particles
    - ▪ Lost energy is *deposited* in the detector material
      - – *Active* materials allow us to detect the energy: e.g. scintillator
      - – *Passive* materials absorb energy without emitting detectable signals: e.g. metal absorbers
  - o Some long-lived particles can also *decay*



- Types of interactions include ionization, electromagnetic physics, hadronic physics, nuclear interactions
  - o GEANT4 can also simulate other types of interactions, such as optical
    - ▪ Not frequently used (computationally expensive), but useful for design (light collection efficiency)

Ionization



- Any charged particle can interact via ionization:

$$\left\langle -\frac{dE}{dx} \right\rangle = Kz^2 \frac{Z}{A}\frac{1}{\beta^2}\left[\frac{1}{2}\ln\frac{2m_e c^2\beta^2\gamma^2 W_{\max}}{I^2} - \beta^2 - \frac{\delta(\beta\gamma)}{2}\right]$$

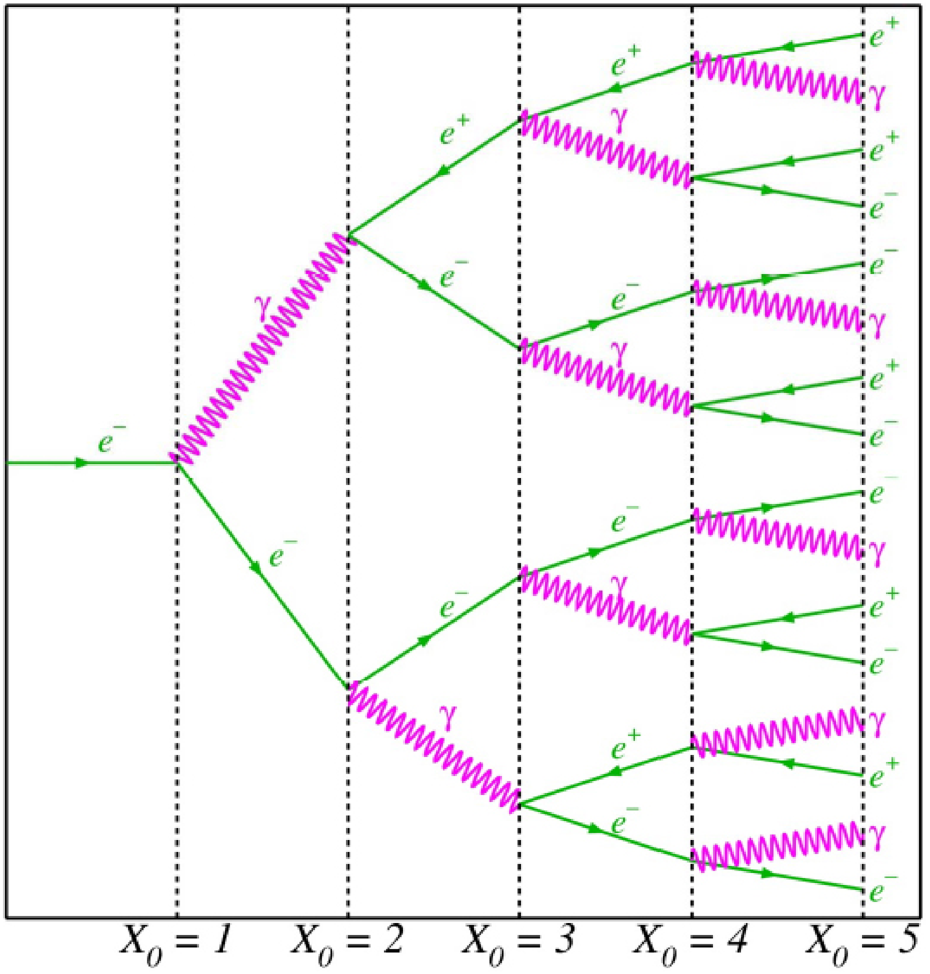
  (Bethe-Bloch formula)
  - o Depends on particle and material properties
- Muons interact almost exclusively via ionization
  - o "Minimum ionizing particles" or MIPs
  - o High-energy muons can emit photons (bremsstrahlung, or "braking radiation")
- Other high-energy particles ionize until they start to *shower*
  - o Low-energy particles mostly deposit energy via ionization

EM Showers

- Electromagnetic (EM) particles include electrons and photons
- For high-energy EM particles interacting with materials:
  - Electron emits a photon (bremsstrahlung)
  - Photon pair produces into two electrons
- These processes occur at very regular intervals: *radiation length* X_0, approximately:

$$1/X_0 = \frac{4\alpha N_A Z(Z+1) r_e^2 \log(183 Z^{-1/3})}{A}$$

  - Electron loses (1 – 1/e) energy after 1 X0
  - Mean free path for photon pair production is $\frac{9}{7}X_0$



EM Showers

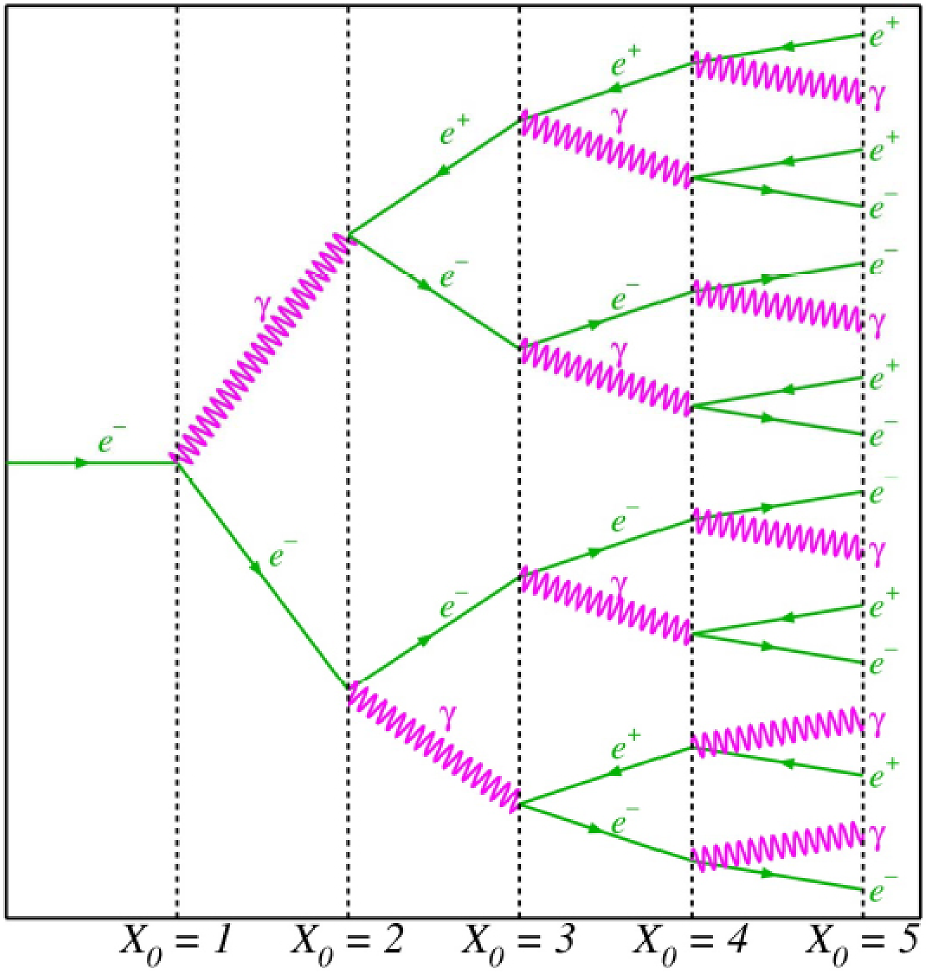
- Transverse size of an EM shower is described by the Molière radius $R_m = E_S X_0 / E_c$
  - Critical energy:

$$E_c = 2.66 \left(X_0 \frac{Z}{A} \right)^{1.1}$$

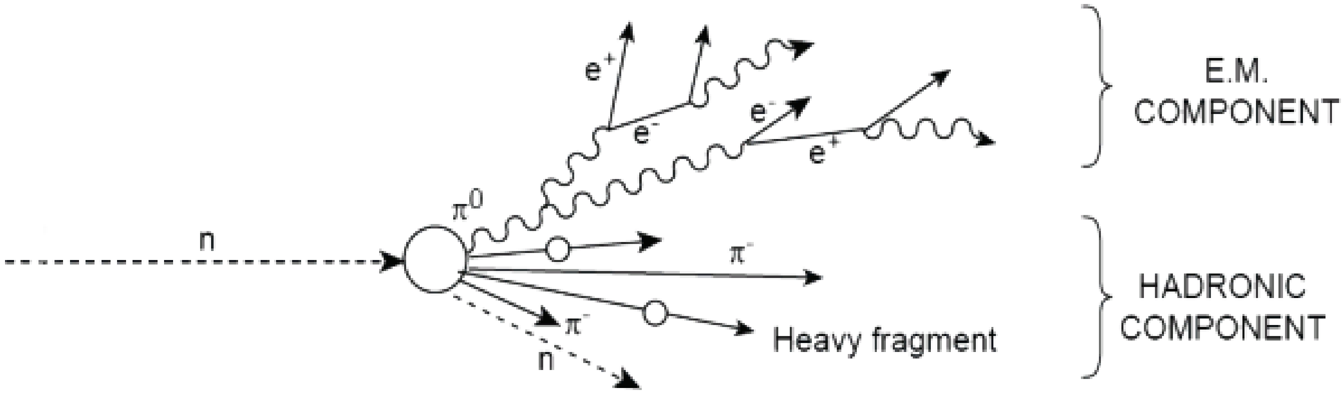
    - bremsstrahlung above, ionization below
  - Scale energy:

$$E_S = \sqrt{\frac{4\pi}{\alpha}} m_e c^2 = 21.2\,\mathrm{MeV}$$

    - from multiple scattering theory
- As energy decreases, other processes take over: Compton scattering, Rayleigh scattering, multiple scattering
  - GEANT4 has different empirical models of these processes for different energy ranges



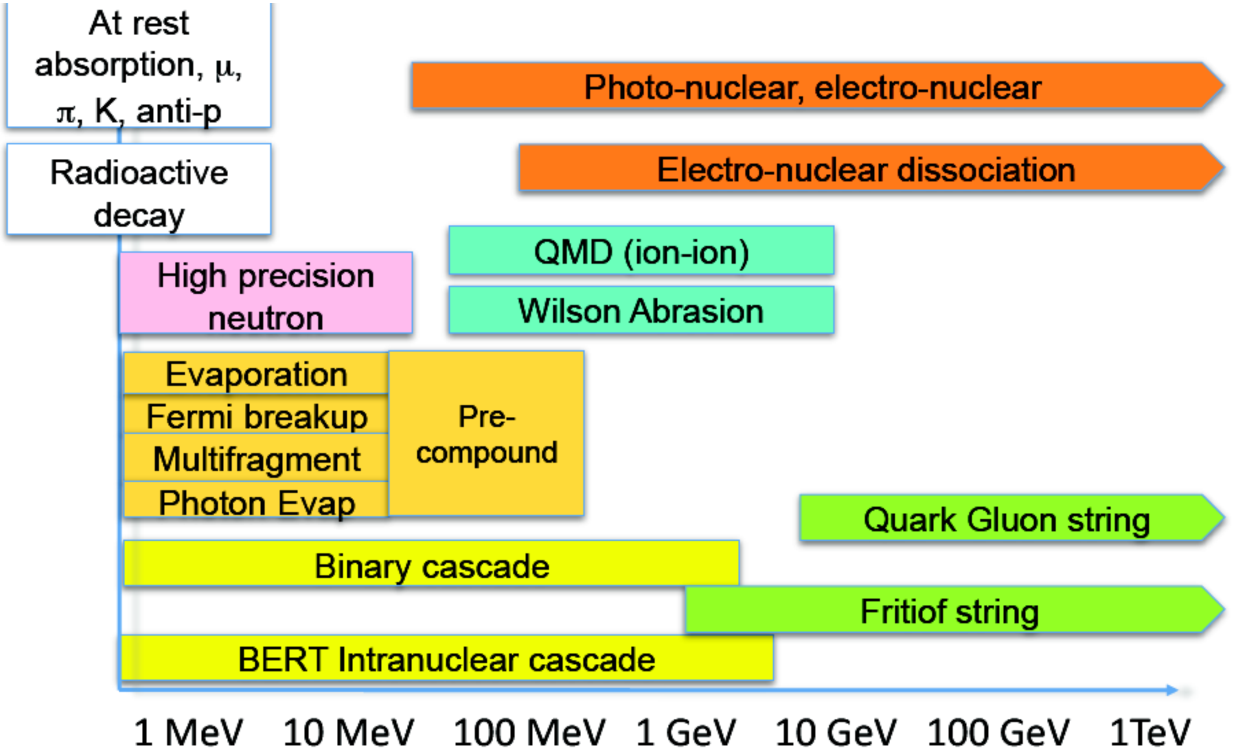
Hadronic Showers



- Highly variable (compared to EM showers)
- Longitudinal and transverse extents both characterized by *interaction length* $\lambda_0 >> X_0$:

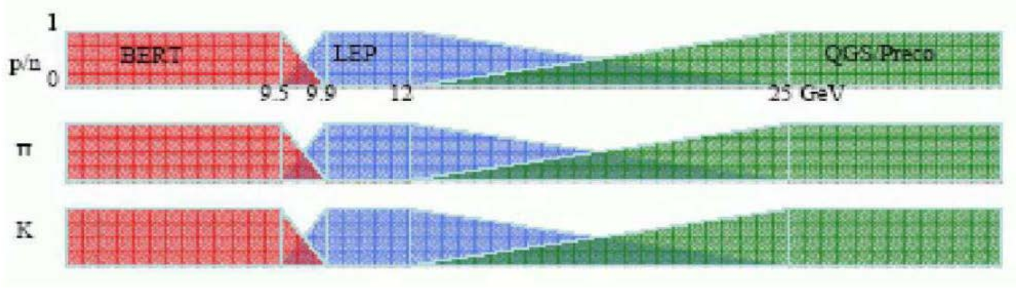
$$\lambda_0 = \frac{A}{\sigma_I N_A} \approx 53(A)^{1/3}$$

- High energy: QGS and FTF models
- Intermediate energy: resonance and cascades, BIC and BERT models
- Low energy: evaporation, etc.
- "Thermal" neutrons have dedicated scattering models
- Most, if not all hadronic physics models are empirical/phenomenological

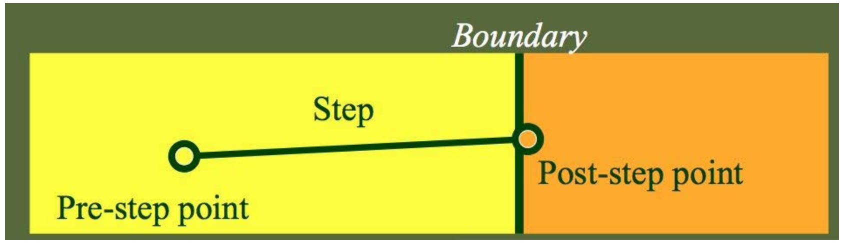


Physics Lists

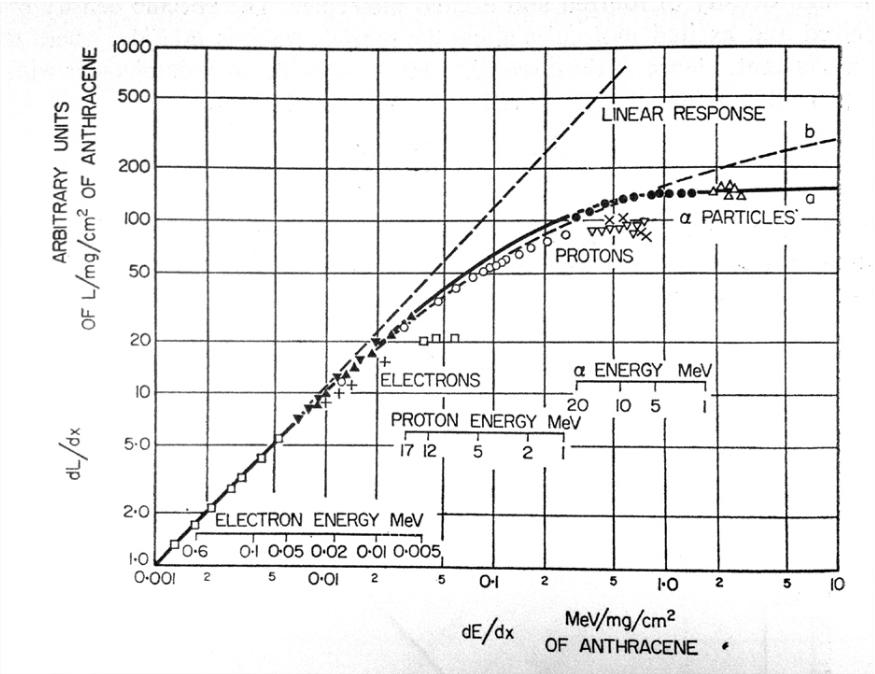
- *Physics list*: a combination of models for physical processes/interactions in various energy ranges
- Some examples of physics lists:
  - QGSP_BERT:
    - Bertini cascade (BERT) at low energies
    - Low energy parameterization (LEP) at intermediate energies
    - Quark gluon string model w/ Pre-compound model (QGSP) at high energies
  - FTFP_BERT
    - Bertini cascade (BERT) at low energies
    - Fritiof model w/ Pre-compound model (FTFP) at high energies
  - Choice of transition region very important!
- Must be combined with a choice of EM physics
  - Different multiple scattering models, etc.



User Actions



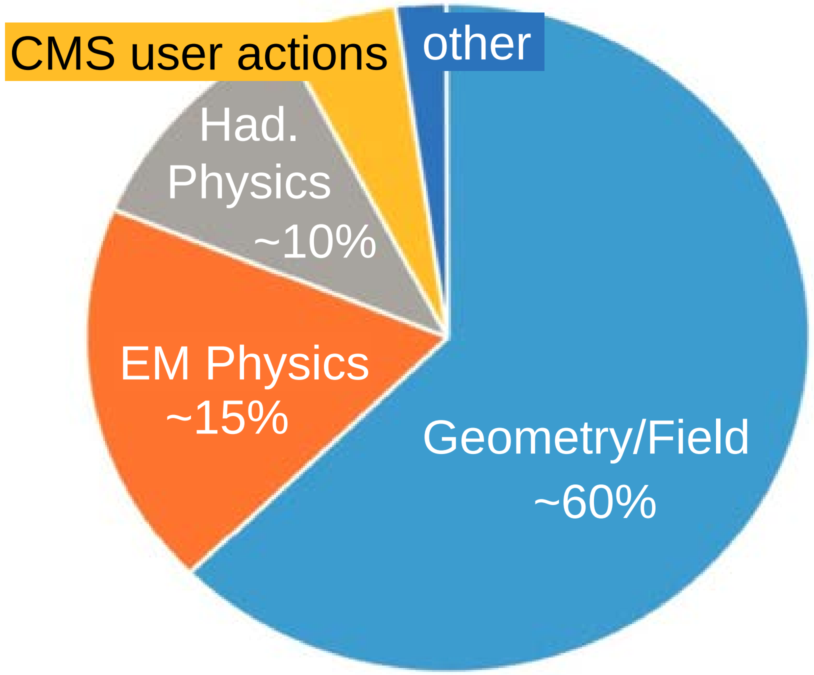
- GEANT4 track represents a particle across multiple steps
  - Each step must be contained within a specific material/volume
  - Each step has two endpoints and an energy deposit in the volume
- Methods available to insert custom actions during any stage (tracking, stepping, etc.)
- Scoring: accumulating/computing physical information, e.g. filling histograms or ntuples
- More sophisticated custom action examples:
  - Creating simulated hits with experiment-specific detector IDs
  - Modifying material responses, e.g. Birks' Law in (organic) scintillators



Controlling GEANT4

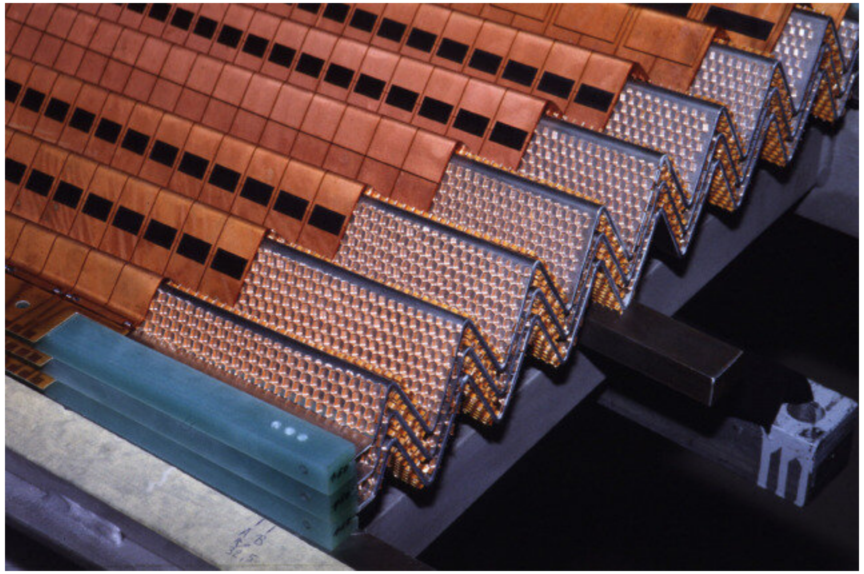
- Many physics processes that produce secondary particles cannot run down to E = 0
  → *infrared divergence* (infinitely many photons at E = 0)
- Such processes are cut off by a *production cut*
  - If a secondary would travel less distance than the production cut, it will not be produced, but rather its energy will just be deposited into the material
  - Distance value can be converted into a material-dependent energy value
- There are also other kinds of cuts:
  - Tracking cut: reject charged particles below some energy in a given volume
    - Prevents looping tracks that take a very long time to evaluate
  - Time cut: maximum propagation time for any particle
- Physics list modifications can also help
  - Many models have their own parameters to tune
  - Can use one model in one region, and a different model in a different region

Speed of GEANT4



Geant4 10.0p02
(similar in other versions)

- For LHC experiments, GEANT4 consumed 40% (*plurality*) of grid computing time during Run 2
- Taking CMS as a case study: largest contributors are geometry, magnetic field, EM physics
- Using default settings, simulating a single $t\bar{t}$ event takes ~80 seconds on a typical CPU
- ATLAS simulation suffers from complicated "accordion" calorimeter geometry → even slower



Speeding up GEANT4

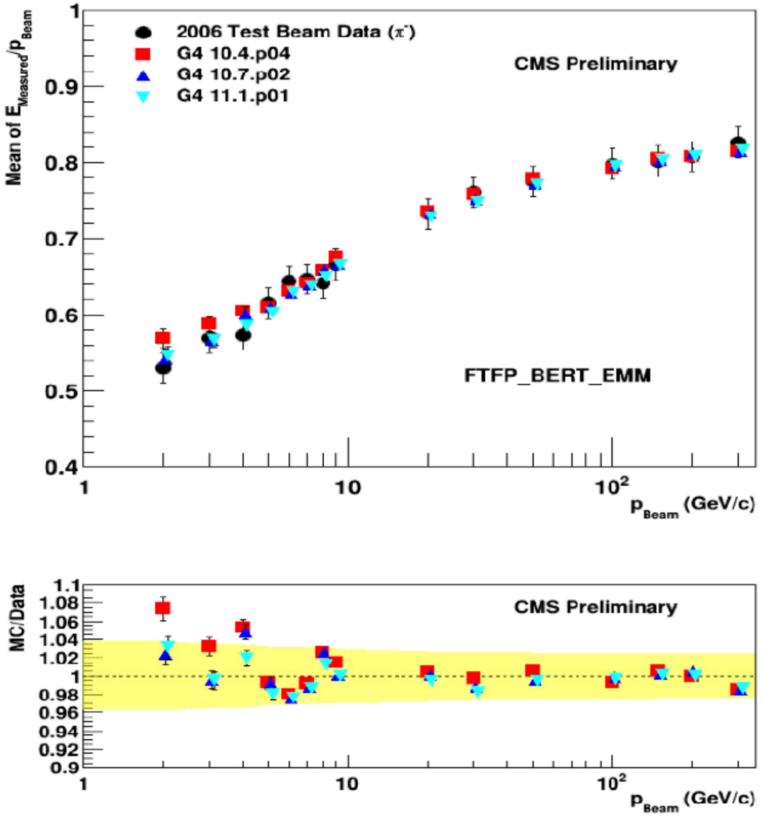
- CMS uses cuts as well as other modifications to speed up the simulation
  - Using latest GEANT4 version also usually helps – collaboration is dedicated to improving the speed!
- *Technical*:
  - Static library: avoid dynamic loading costs
  - VecGeom: newer geometry engine w/ more efficient code
  - Magnetic field: newer G4DormandPrince745 algorithm uses fewer evaluations, plus energy-dependent tracking
- *Approximations*:
  - Shower library: high multiplicity of particles in forward region ($|\eta| > 3$), use pre-generated showers instead
  - Russian roulette: discard N-1 low-energy neutrons or photons and give the N^{th} particle a weight of N
  - FTFP_BERT_EMM: modified physics list w/ simplified multiple scattering in most regions (except HCAL)

➢ Cut $t\bar{t}$ simulation down to ~20 s/evt!

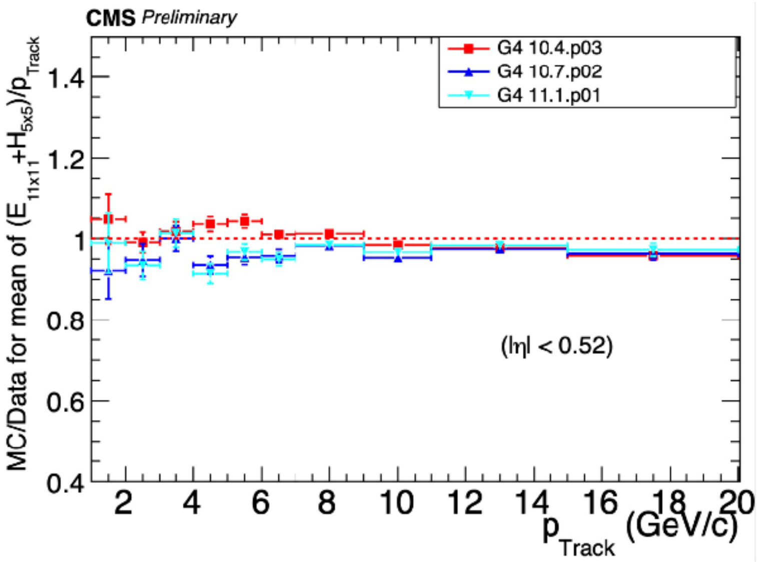
	Relative CPU usage	
Configuration	**MinBias**	**ttbar**
No optimizations	1.00	1.00
Static library	0.95	0.93
Production cuts	0.93	0.97
Tracking cut	0.69	0.88
Time cut	0.95	0.97
Shower library	0.60	0.74
Russian roulette	0.75	0.71
FTFP_BERT_EMM	0.87	0.83
VecGeom (scalar)	0.87	0.93
Mag. field step,track	0.92	0.90
All optimizations	0.16	0.24

Validating GEANT4

- New versions, approximations, etc. improve speed – but need to ensure physics is not harmed
- Multiple sources of validation data (shown below)



2006 test beams: known beam properties, dedicated geometry implementation



Isolated tracks from low-pileup collision runs: require charged tracks, neutral energy clusters to have minimal surrounding activity

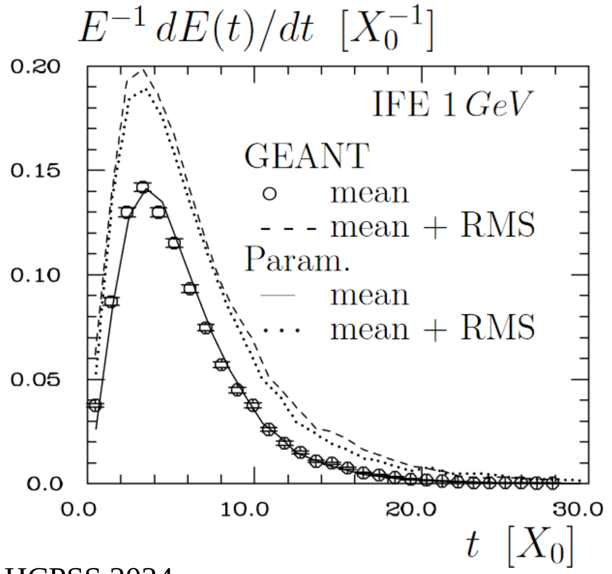
➢ Once these tests pass, new GEANT4 version is validated at larger scale by producing full MC samples

Faster Simulation

- Can we avoid modeling every interaction, tracking every secondary particle, etc.?
- One approach: GFLASH, parameterize behavior of particle showers
  - Works especially well for EM showers (more regular)
  - Parameters as function of energy from fitting GEANT4 output
    - Fluctuations in parameters also modeled

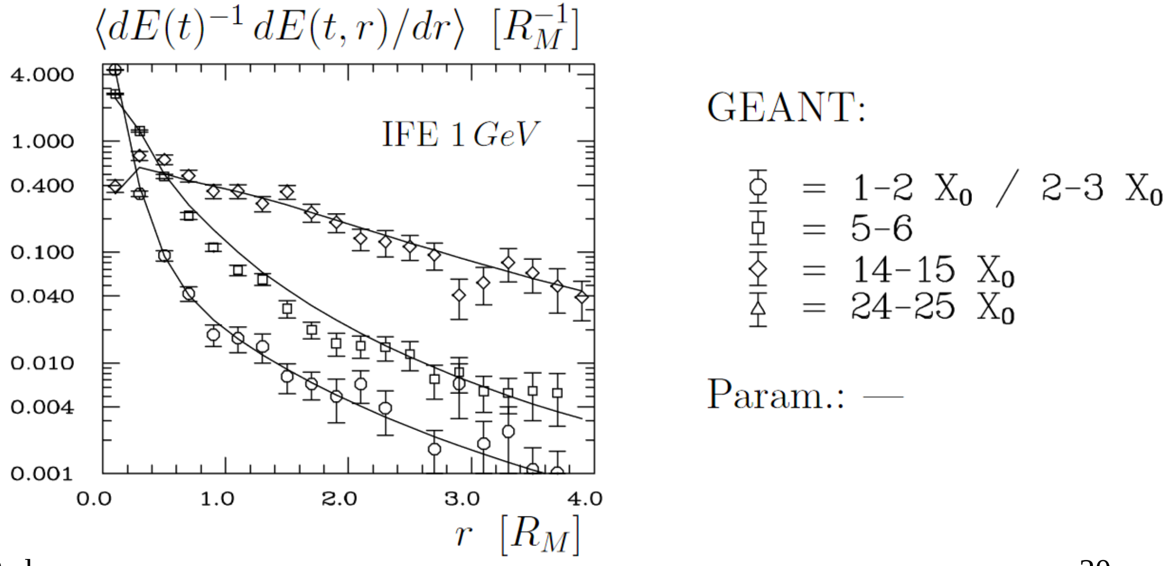
Longitudinal:

$$\left\langle \frac{1}{E}\frac{dE(t)}{dt} \right\rangle = f(t) = \frac{(\beta t)^{\alpha-1}\beta\exp(-\beta t)}{\Gamma(\alpha)}$$



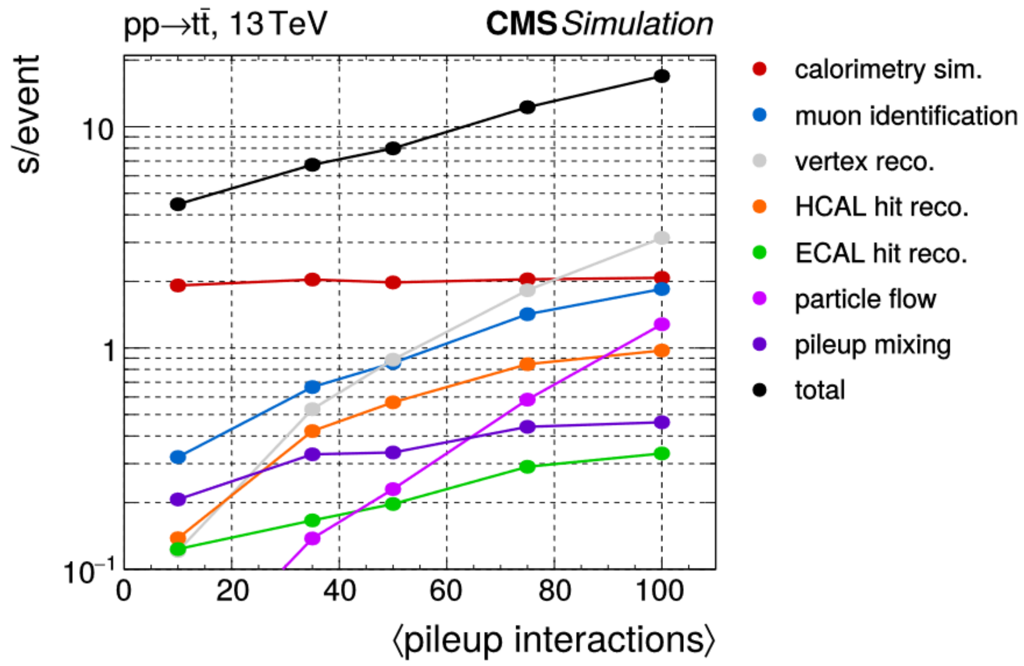
Radial: (core and tail components)

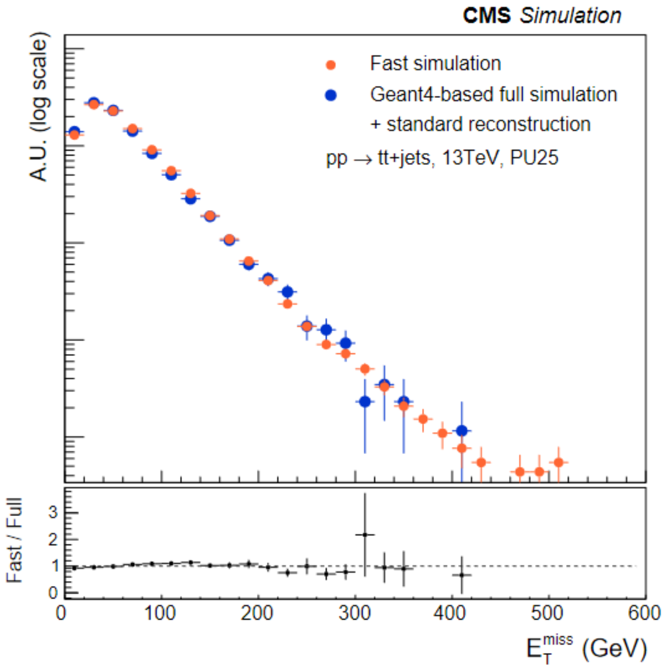
$$\begin{aligned} f(r) &= p f_C(r) + (1-p) f_T(r) \\ &= p\frac{2rR_C^2}{(r^2+R_C^2)^2} + (1-p)\frac{2rR_T^2}{(r^2+R_T^2)^2} \end{aligned}$$



CMS FastSim

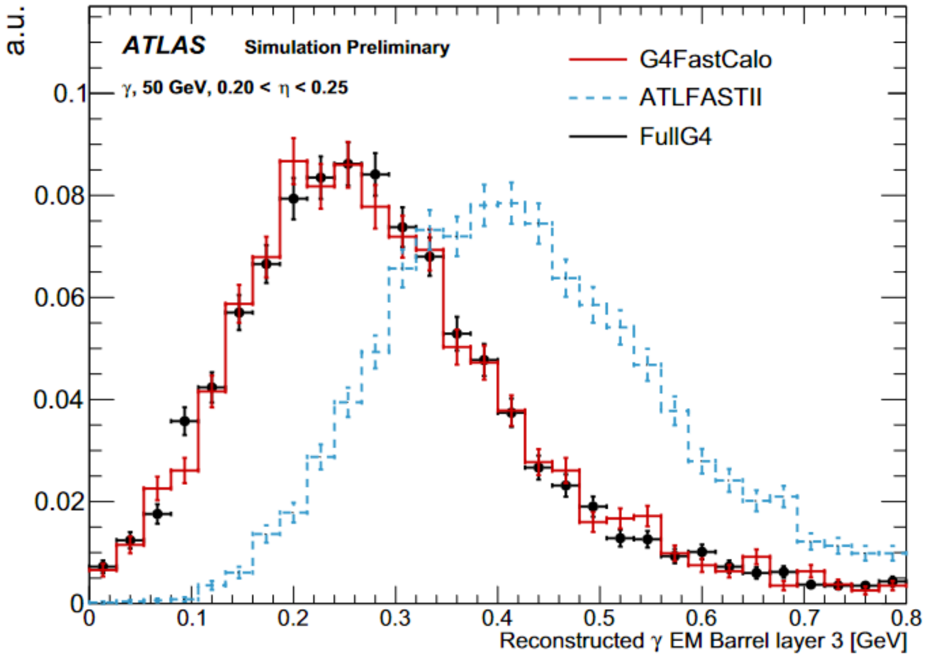
- CMS FastSim uses a combination of techniques:
  - Simplified detector geometry, magnetic field, interactions
  - GFLASH-based parameterizations for particle showers in ECAL and HCAL
  - Shower library for forward region
  - Generator-assisted track finding (reconstruction step)
- Achieves ~100× speedup in SIM step and agreement with GEANT4 within ~10%



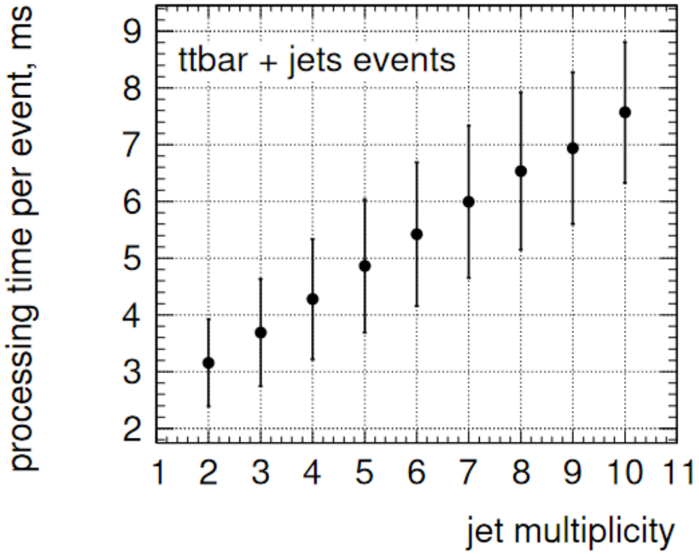


Other Fast Simulations

- ATLAS FastCaloSim:
  - Uses principal component analysis in modeling of energy deposition & longitudinal and radial shower profiles (decorrelate between calorimeter layers)
  - About 10× faster than GEANT4



- Delphes: ultra-fast parametric simulation
  - Applies efficiencies, resolutions, etc. to generator particles
  - Can be tuned to different detectors' performance (based on measurements)
  - Limitations: "fake" objects, instrumental effects missing
    - Pileup can be included
  - Frequently used for phenomenological studies
  - ~few ms to simulate $t\bar{t}$ event: 1000× faster than CMS FastSim



Digitization

- GEANT4 outputs are energy deposits in a detector volume
- These need to be converted into what we *actually detect*: light or charge

➢ Second dedicated *DIGI step* for electronics simulation

  - SIM step depends on geometry, materials → known and fixed once detector is built
  - DIGI step depends on changing conditions: pedestals, radiation damage, etc.
    - Also apply other conditional effects during this step, e.g. pileup mixing

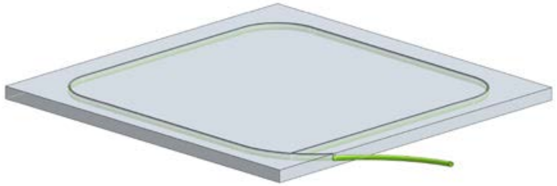
- Usually bespoke implementations
  - Detector electronics are very particular and complicated
  - Example on next slide

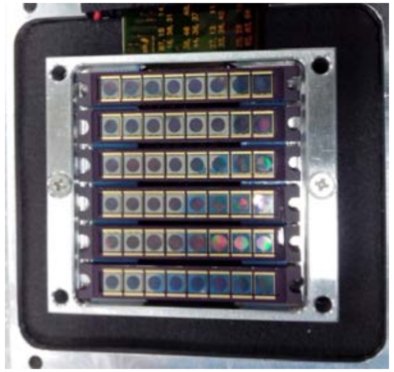
Example: CMS HCAL SiPMs

Randomly sampled
Directly applied

- Silicon photomultipliers: precise single-photon detectors

1. Convert deposited energy to scintillation photons (Poisson photostatistics)
2. Account for rise time of scintillator and wavelength shifting fiber (measured distribution)
3. Add dark current (single photoelectron noise, Poisson)
4. Randomly assign each photon to SiPM pixel (flat)
5. Add cross-talk: pixels inducing discharges in other pixels (Borel-Tanner distribution)
6. Account for pixel saturation and recovery (exponential)
7. Apply SiPM pulse shape to pixels (measured distribution)
8. Convert to charge and add pedestal from QIE: charge integrator and encoder (Gaussian)
9. Apply time slew from QIE (measured distribution)

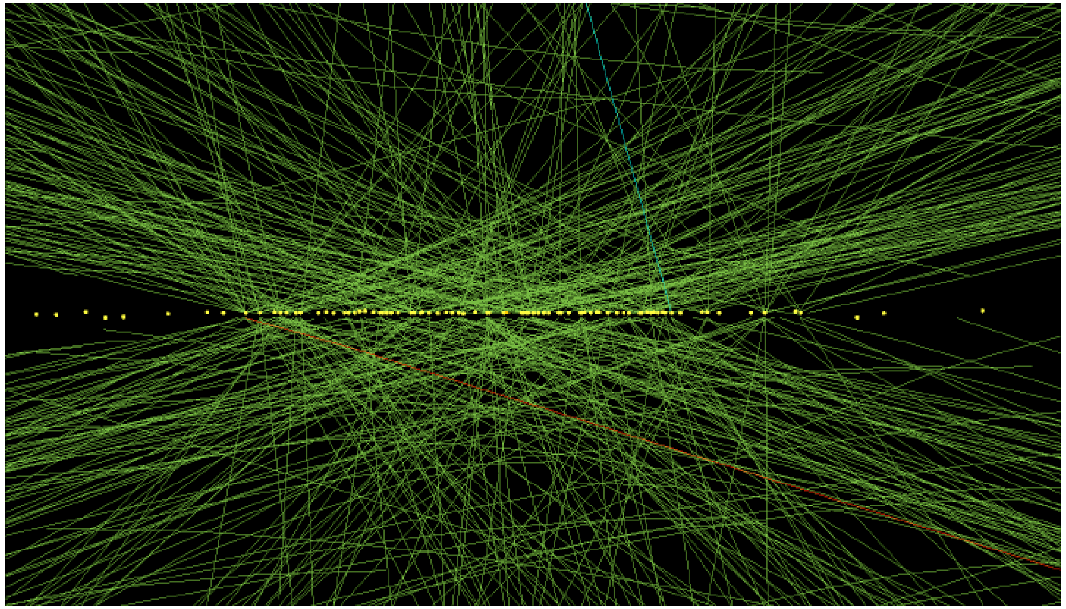




➢ An entire mini-MC for *each detector*!

- During this process: can also apply radiation damage to scintillator (darkening) and SiPM (dark current increase) as functions of luminosity (based on measurements)

Pileup Mixing

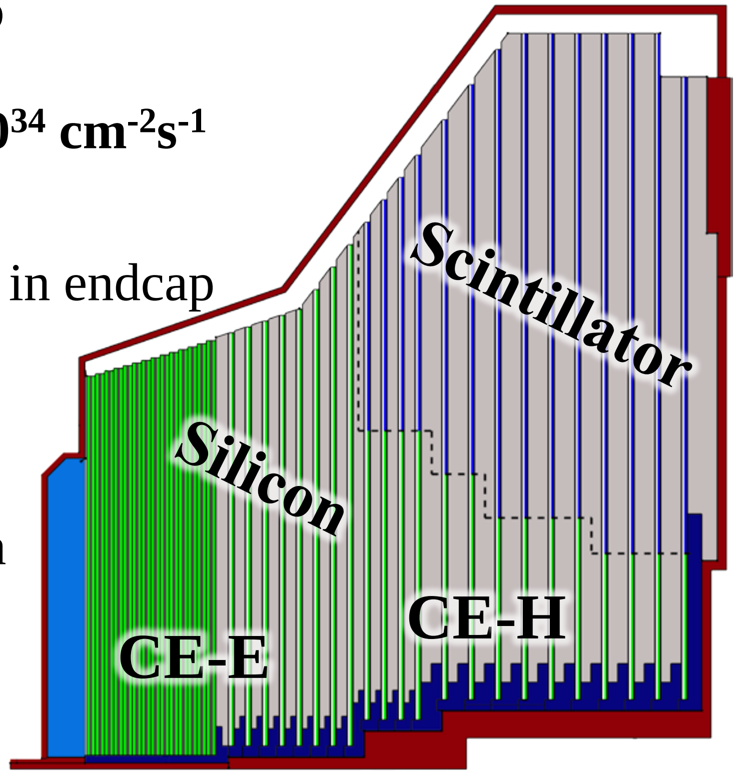


- Pileup: simultaneous pp collisions in a bunch crossing
  - *Not* noise, but rather an *unwanted signal*
- Classical approach: overlay N simulated minimum bias events on signal event
  - We also model additional bunch crossings before and after crossing of interest (total of M crossings)
  - Therefore, this approach requires N×M minbias events for each signal event
- Premixing: combine N minbias events in advance
  - Naïve approach not good enough: still carrying around N events' worth of simulated hits
  - Run a partial version of DIGI step to compress into pseudo-digitized formats
    - e.g. for SiPMs: just perform steps 1, 2 → store "photons" (with highly granular time binning)
  - During signal DIGI step, overlay just 1 premixed event (combining as appropriate) → M total

➢ Substantial improvement over classical mixing
  - But still requires hosting multiple copies of O(PB) datasets and serving throughout the grid

HL-LHC Challenges

- High Luminosity LHC will have an instantaneous luminosity of **5–7.5×10^{34} cm^{-2}s^{-1}**
  → more **data**, more **radiation**, more **pileup** (~140–200)
- CMS detector upgrades including High Granularity Calorimeter (HGCal) in endcap
  - ~6 million channels (vs. ~100K channels currently)
- Simulating HGCal requires 10× more geometry volumes
- Also requires more accurate physics lists to match measurement precision
  - **FTFP_BERT_EMN**:
    - Goudsmit-Saunderson model for multiple scattering below 100 MeV
    - Angular generator for bremsstrahlung
    - More accurate Compton scattering model

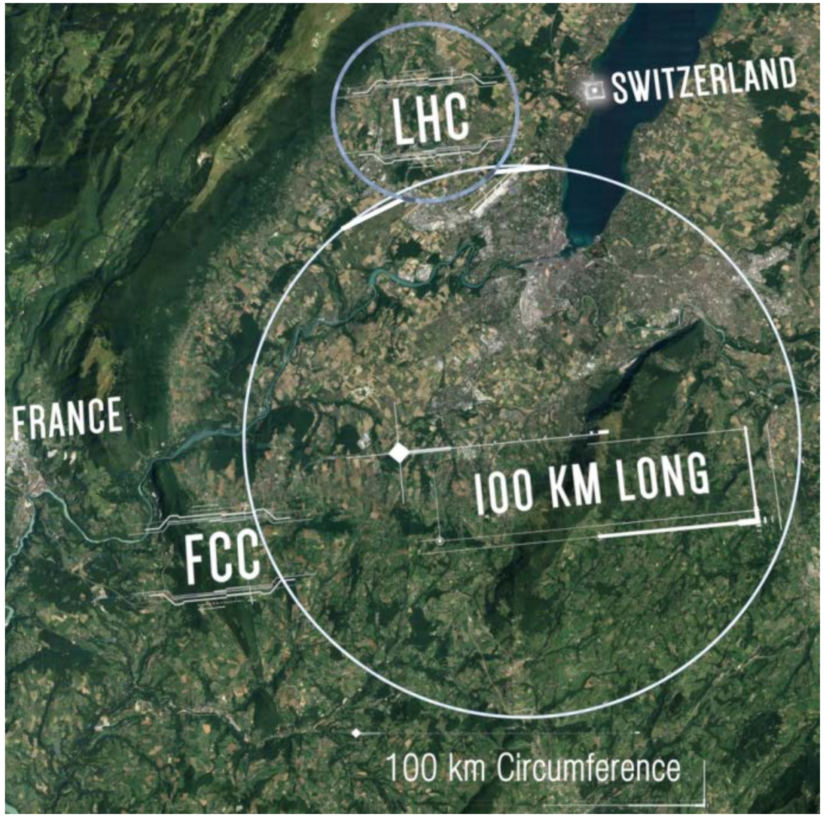


➢ Simulation takes **2–3×** longer w/ new geometry & physics list

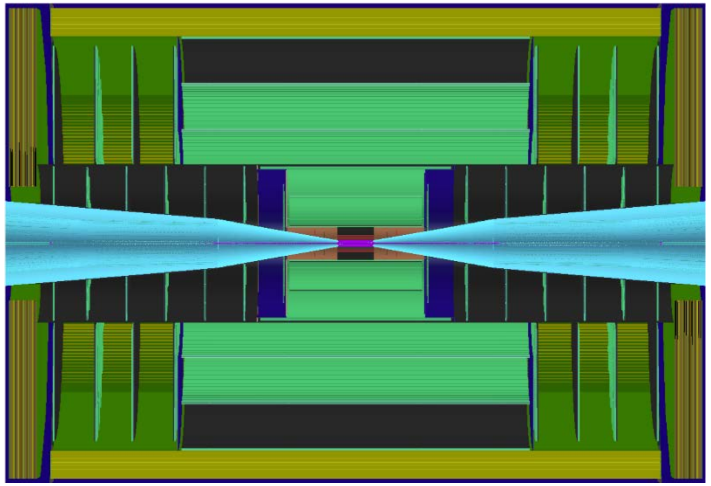
		Run 2	Run 4 (range)	
Minimum Bias	**FTFP_BERT_EMM**	1.00	1.18	1.24
(10.5.ref08)	**FTFP_BERT_EMN**	1.06	2.01	2.15
ttbar	**FTFP_BERT_EMM**	1.00	1.64	1.75
(10.5.ref08)	**FTFP_BERT_EMN**	1.14	2.97	3.25

Future Collider Challenges

- **FCC-hh**: ~100 km ring, $\sqrt{s_{pp}} \approx 100$ TeV
  - Expected pileup 1000: 2.5×10^5 > 100 MeV
  - *Significant escalation* from previous slide

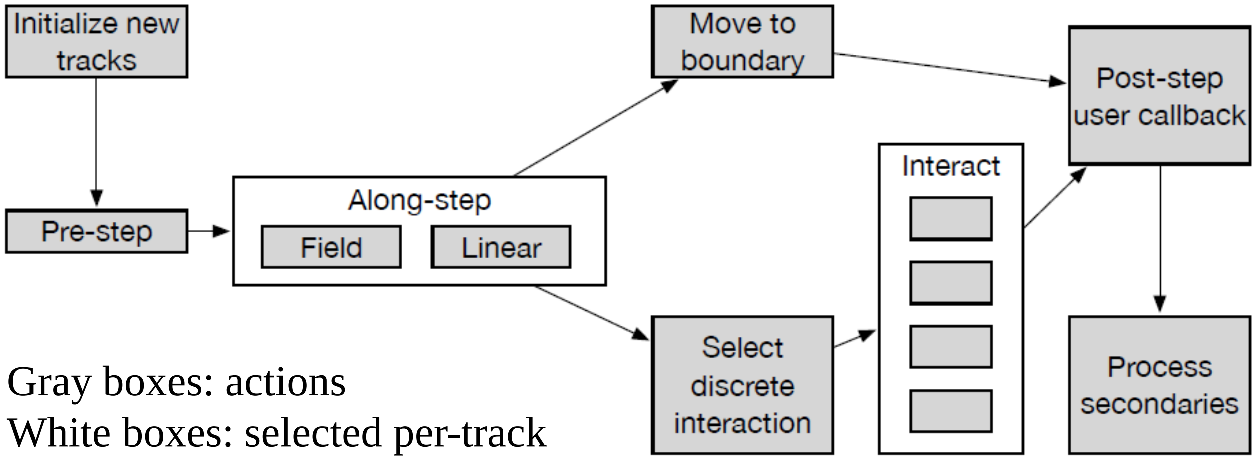


- **Muon Collider**: ~16 km ring, $\sqrt{s_{\mu\mu}} \approx 10$ TeV (≈70–150 TeV in $\sqrt{s_{pp}}$,)
  - *Beam-induced background*:
    - ~10^5 muon decays per meter
    - ~10^8 photons and neutrons per crossing
    - ➢ *24 hours* to simulate 1 event in Geant4
  - Designing & optimizing machine-detector interface (e.g. tungsten nozzle) requires substantial intensive simulation

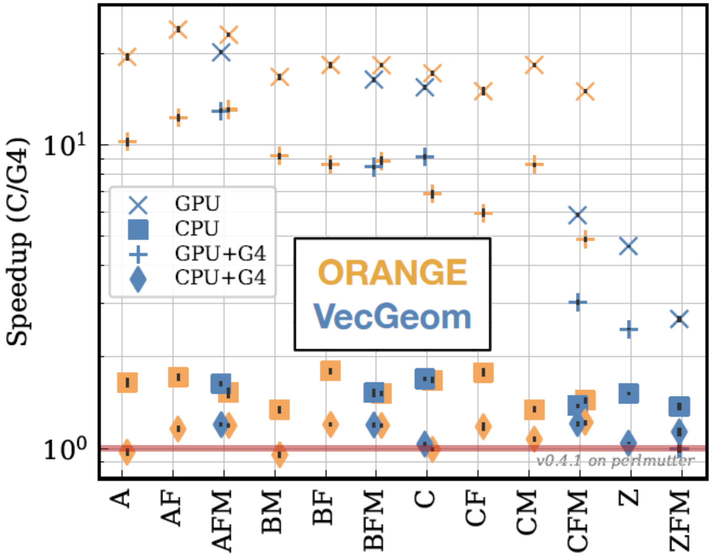


GPU Simulation

- Graphics processing units (GPUs) can execute certain operations much faster than CPUs
  - o Need to use domain language like CUDA, w/ SIMD (single instruction, multiple data) paradigm
  - ➢ Process tracks *in parallel* while allowing each track to take random action
- *Celeritas* project is addressing this
  - o Reimplement major components for GPU: geometry, magnetic field, EM physics
  - o Can reuse GEANT4 interfaces for user actions; run standalone or offload from within GEANT4



Gray boxes: actions
White boxes: selected per-track



- Results in various scenarios: speedup even for CPU-only!
  - o New geometry engine ORANGE outperforms VecGeom on GPU
- In progress: more physics processes (neutrons, hadrons, etc.)
- Other related projects:
  - o Opticks (optical only), AdePT/G4HepEM (EM only, w/in GEANT4)

Conclusions

- Simulation is critical for HEP, with numerous elements:
  - Geometry construction & navigation, magnetic field propagation, material properties, particle interactions, electronics responses, pileup
  - Need to understand a wide range of physics, as well as computing to ensure efficiency
- GEANT4 is the state of the art
  - Constant work to improve both physics and computing performance
  - Numerous fast approximations exist, with varying levels of speed and accuracy
  - New GPU-based simulations are promising to move beyond incremental speedups
- Upcoming experiments present special challenges for simulation
- Are there other ways to speed up simulation?
  - How about machine learning?
  - Stay tuned…

Backup

References

- Geant4 manuals: https://geant4.web.cern.ch/docs/
- X International Geant4 School
- PDG, "Passage of particles through matter", https://pdg.lbl.gov/2024/reviews/rpp2024-rev-passage-particles-matter.pdf
- N. Srimanobhas et al., "Full Simulation of CMS for Run-3 and Phase-2", EPJ Web Conf. 295 (2024) 03017.
- HEP Software Foundation, "Detector Simulation White Paper", https://arxiv.org/abs/1803.04165.
- S. Sekmen, "Recent Developments in CMS Fast Simulation", PoS ICHEP2016 (2016) 181.
- M. Komm, "Fast emulation of track reconstruction in the CMS simulation", J.Phys.Conf.Ser. 898 (2017) 042034.
- G. Grindhammer, M. Rudowicz, and S. Peters, "The Fast Simulation of Electromagnetic and Hadronic Showers", https://inspirehep.net/literature/281126.
- G. Grindhammer and S. Peters, "The Parameterized Simulation of Electromagnetic Showers in Homogeneous and Sampling Calorimeters", https://arxiv.org/abs/hep-ex/0001020.
- J. Schaarschmidt, "Upgrading the Fast Calorimeter Simulation in ATLAS", https://www.osti.gov/servlets/purl/1544173.
- J. de Favereau et al., "DELPHES 3, A modular framework for fast simulation of a generic collider experiment", JHEP 02 (2014) 057.
- S. Banerjee, "Validation of Physics Models of Geant4 using Data from CMS Experiment", J. Phys.: Conf. Ser. 898 (2017) 042005.
- Geant4 Hadronic Working Group, "Improvements in the Geant4 Hadronic Physics", J. Phys.: Conf. Ser. 331 (2011) 032002.
- CMS HCAL Collaboration, "Brightness and uniformity measurements of plastic scintillator tiles at the CERN H2 test beam", JINST 13 (2018) P01002.
- M. Mangano et al., "Conceptual design of an experiment at the FCC-hh, a future 100 TeV hadron collider", CERN-2022-002.
- J. P. Delahaye et al., "Muon Colliders", arXiv:1901.06150.
- K. Black et al., "Muon Collider Forum report", JINST 19 (2024) T02015.
- Muon Collider Collaboration, "Simulated Detector Performance at the Muon Collider", arXiv:2203.07964.
- S. Johnson et al., "Celeritas R&D Report: Accelerating Geant4", https://info.ornl.gov/sites/publications/Files/Pub206160.pdf.