# The Geant4 toolkit for the simulation of high luminosity experiments

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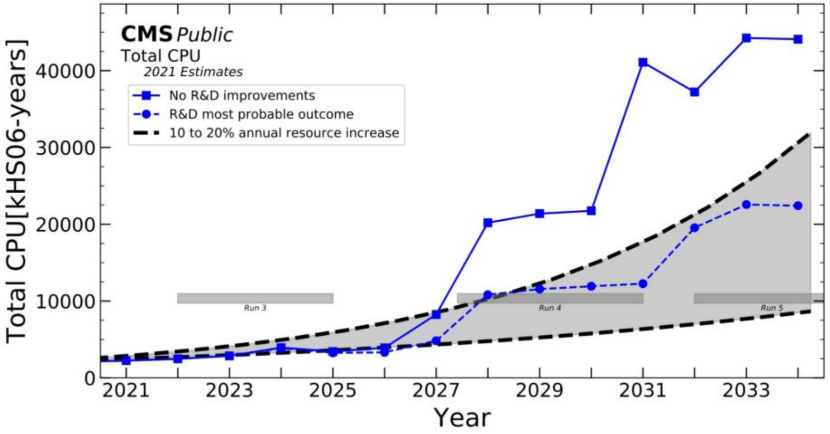
# Outline

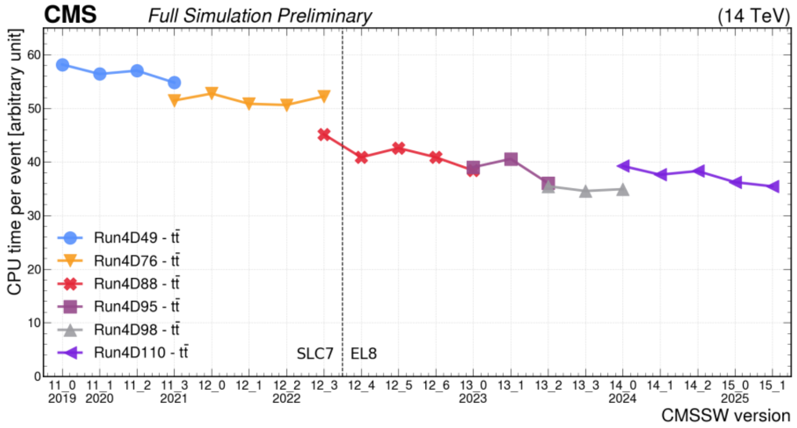
- Geant4 toolkit
  - Current main challenges
- Geant4 EM physics
  - Electromagnetic physics
  - Simulation of channeling
  - DNA physics and Chemistry
- Geant4 Hadronic physics
- Medical physics benchmark
- R&D for Phase2 LHC
  - G4HepEm library
  - AdePT and Celeritas projects
- What is expected in 2025 release
- Conclusions

- Geant4 History
  - Dec ’94 –R&D project start
  - Dec ’98 -First Geant4 public release -version 0.0
- 2004: ATLAS, CMS, and LHCb start using Geant4
- Dec 2013 – version 10.0 – 1st with multi-threading
  - Dec 2020 - version 10.7 completed 10 series
- Dec 2021 – Geant4 11.0 – start of the new series
  - Dec 2024 – Geant4 11.3 – recent public version
- Dec 2025 – expected 11.4
  - June 2025 11.4beta available for users
- Main publications (citations checked 17.08.2025)
  - Nucl. Instr. Meth. A 506, 250-303 (2003 ) cited 20708
  - IEEE Trans. Nucl. Sci. 53, 270-278 (2006) cited 4516
  - Nucl. Instr. Meth. A 835, 186-225 (2016) cited 2105
  - Medical Physics 45, e722–e739 (2018) cited 452
  - Medical Physics, 48, 19-56 (2021) cited 199

# Main challenges

- The Geant4 toolkit is the main Monte Carlo simulation tool for the Large Hadron Collider (LHC) experiments
  - Total number of events generated over $10^{10}$.
  - LHC Run3 will be completed in 2026
- Run4 will operate at significantly higher luminosity and generate substantially more data
  - The main task for all LHC experiments is to prepare software, which will be capable to handle significantly more experimental data.
    - J. Apostolakis et al., Front.in Phys. 10 (2022) 913510
  - Geant4 simulations must be updated in terms of physics model accuracy and CPU performance to meet the demands of the new phase.
    - Both ATLAS and CMS teams already implemented several improvements, which in sum provide ~factor 2 speed-up versus Run-2
    - The next possibility is to utilise Geant4 at GPU



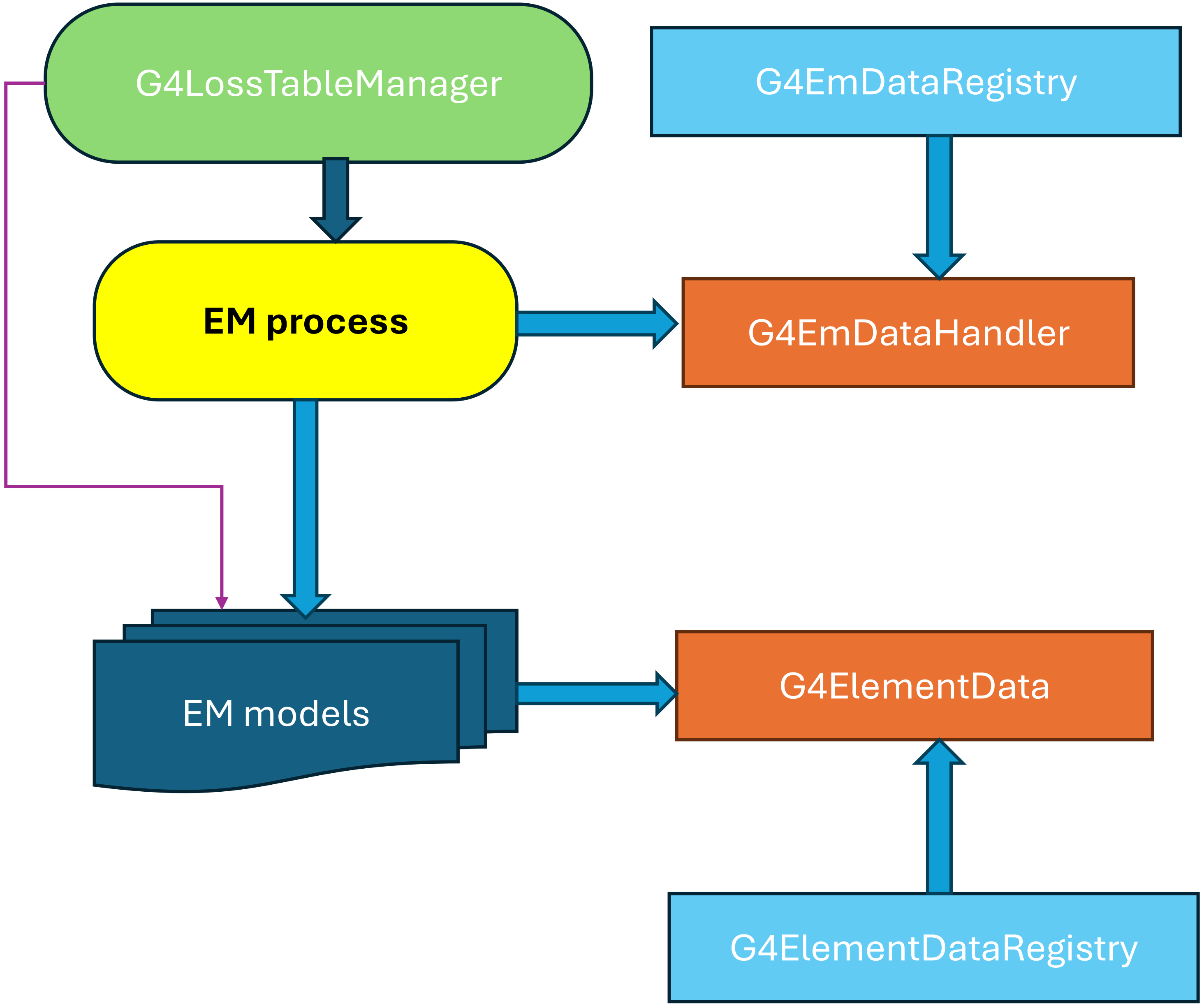



# Electromagnetic (EM) physics developments

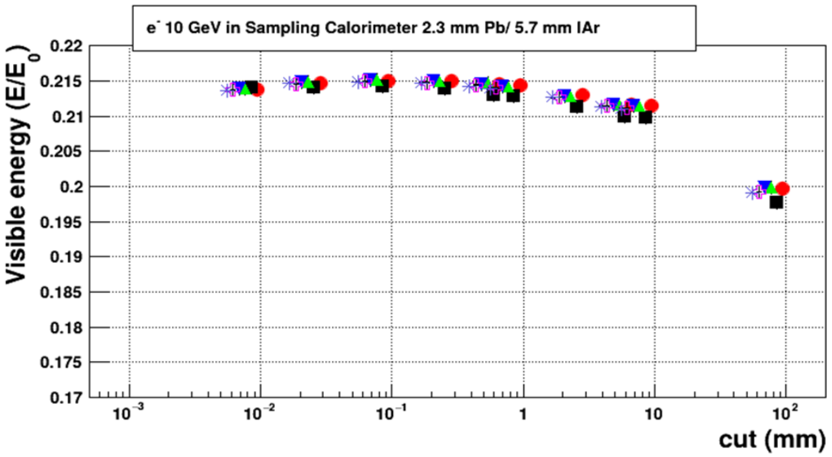
- Predictions for EM shower shape in HEP calorimeters are stable on level $10^{-3}$ since Geant4 10.5
  - Some efforts were carried out to improve infrastructure and user interface to EM physics
- Important updates were introduced with Geant4 10.6
  - Fixed LPM effect description for bremsstrahlung
  - Theory based GS model of e+- multiple scattering
  - These models are essential for recent studies of ATLAS EM shower shape and CMS HGCal calorimeter response
- Main developments for HEP are carried out to add next to leading order corrections and addition of rare processes
  - 5D models for gamma conversion in e+e- or $\mu^+\mu^-$ pairs
  - Alternative 5D model for e+e- pair production important for $\mu$e scattering experiment
  - Production of $\mu^+\mu^-$ pairs by muons
  - 2- and 3- gamma positron annihilation including positronium formation
  - Ionisation and multiple scattering for “unknown” changed particles
- Models important for developments of future facilities
  - Transport of linear polarized photons
  - EM physics in crystals
  - X-rays processes for accelerators
  - Cerenkov and scintillation redesign – handling of alternative models for different sub-detectors
- Low-energy models MicroElec and DNA
- Below some examples of new developments will be shown

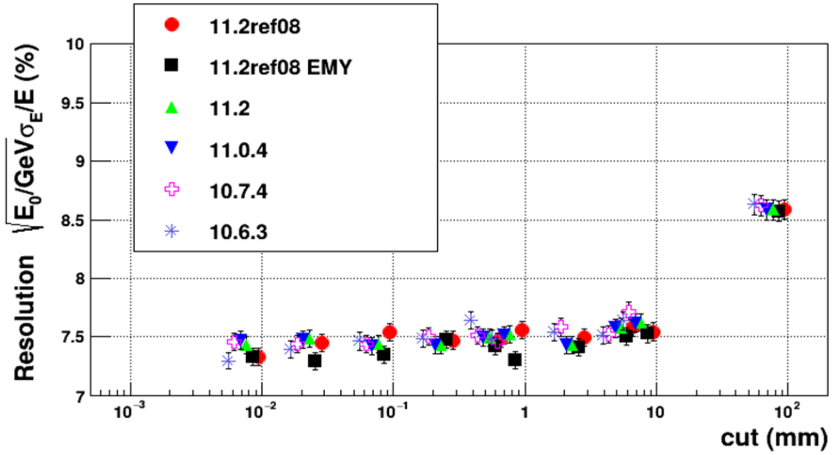
# EM data handling since Geant4 11.3

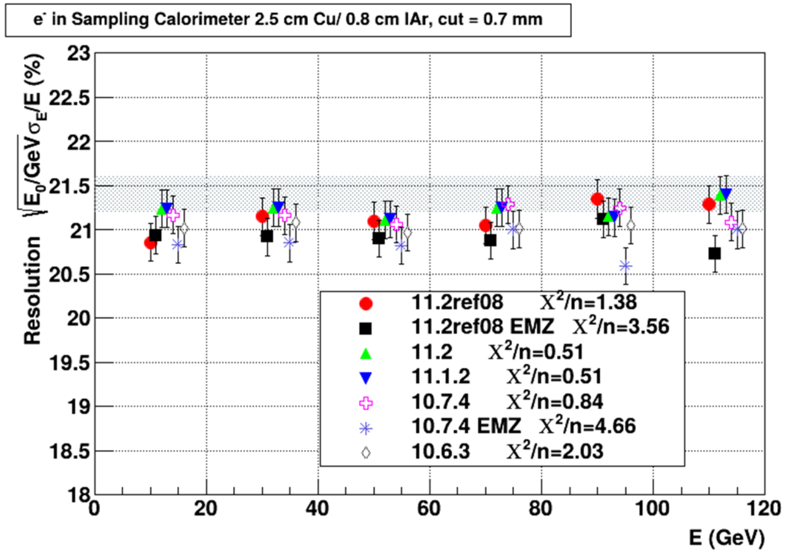
- G4LossTableManager define master thread in constructor
  - It may be the first working thread
  - Data structures are shared between threads
- G4ElmentDataRegistry keeping G4ElementData for EM models
  - Cross sections per element
  - Sampling tables
  - It is responsible for data deletion end of job
- G4EmDataRegistry keeping shared data from EM processes
  - Physics tables
  - EM cross section shape data
  - It is responsible for data deletion end of job

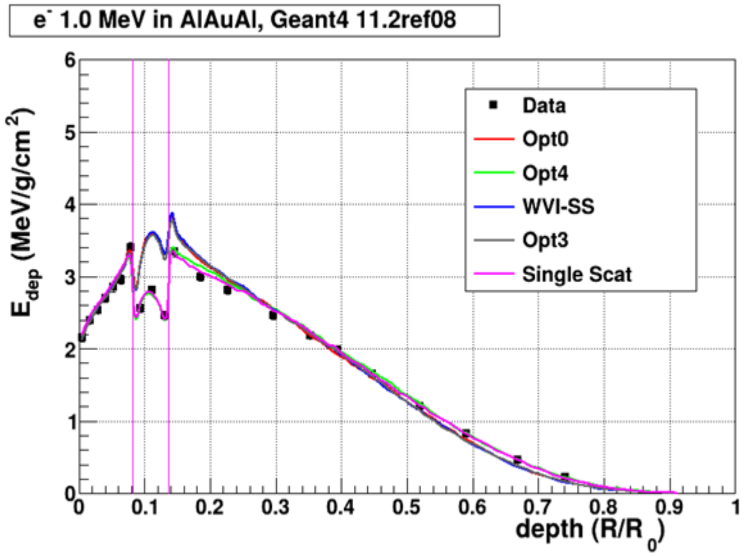


# Recent validation results

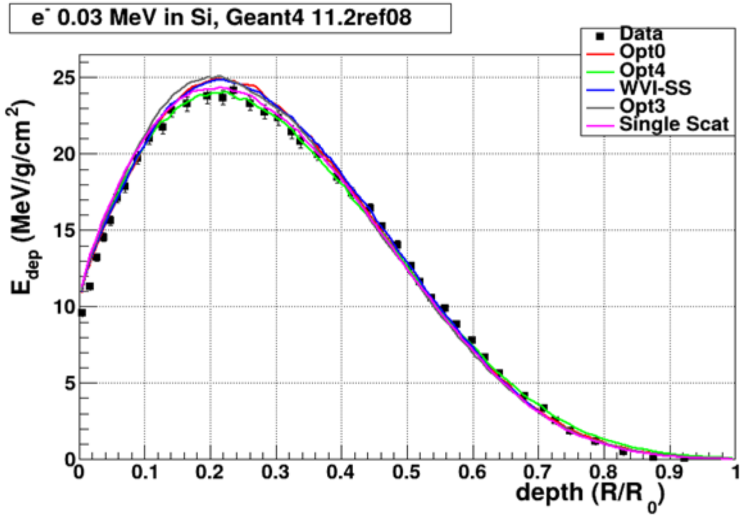


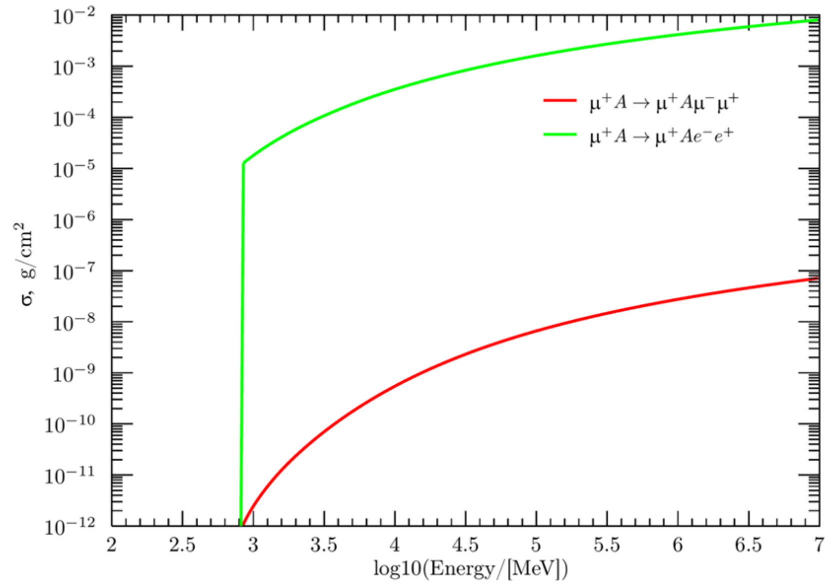



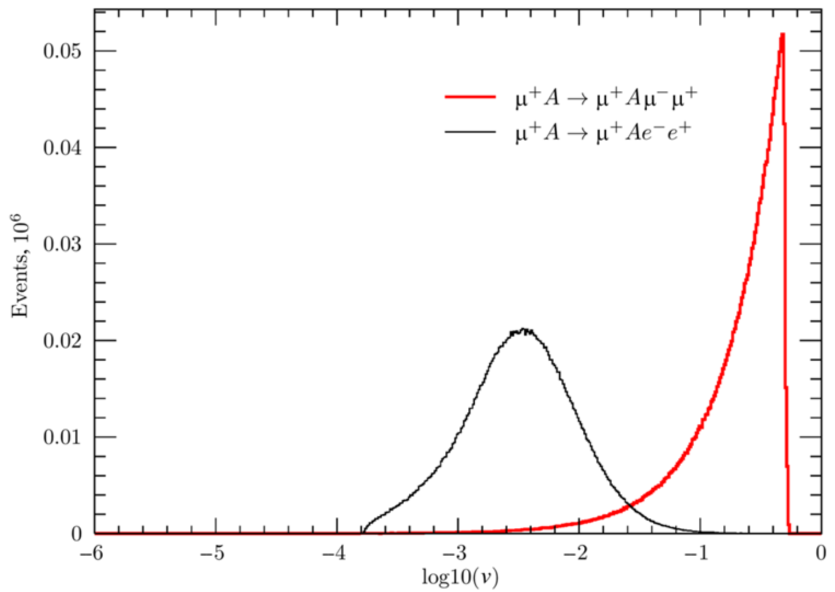

- There is stability in for EM calorimetry response simulation from 10.6 to 11.3
  - Mean energy deposition and its width are unchanged within statistical fluctuations
  - The only known unstable EM physics is EMY for protons, which was fixed in 11.2.2



# Muon pair production by muons

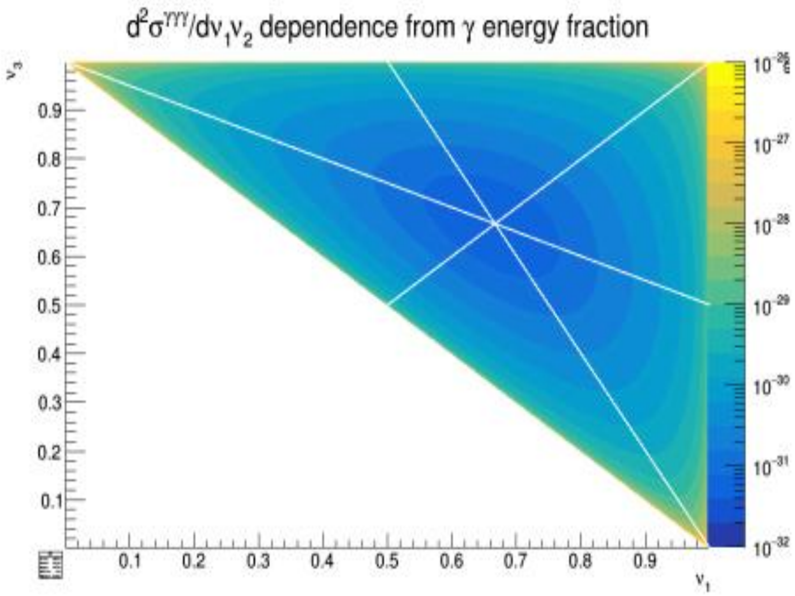
- Observed in BARS and ALEPH experiments
- Relevant to ATLAS and CMS
  - Important for SND@LHC forward ATLAS experiment
    - Still problems data/experiment – investigation is ongoing
- Cross section is about $10^{-5}$ of e+e- production
  - Final energy of muons is compatible with the primary muon energy – 3 similar muons
    - In contrast to e+e- pair production spectra
- Main publications:
  - S.R. Kelner, R.P. Kokoulin, A.A. Petruhkin, Phys. Atom. Nuclei 63, 1603–1611 (2000).
  - A. Bagulya et al., Russian Physics Journal 67, 2379–2382, (2024)

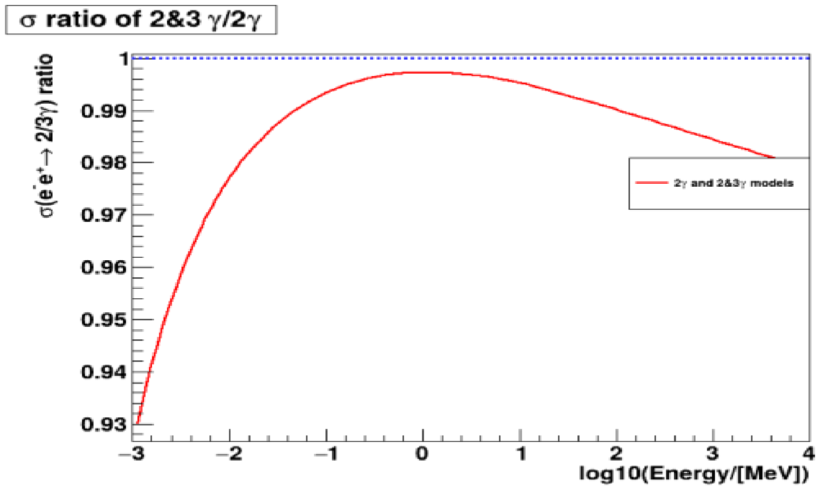


# Positron 2- and 3-gamma annihilation

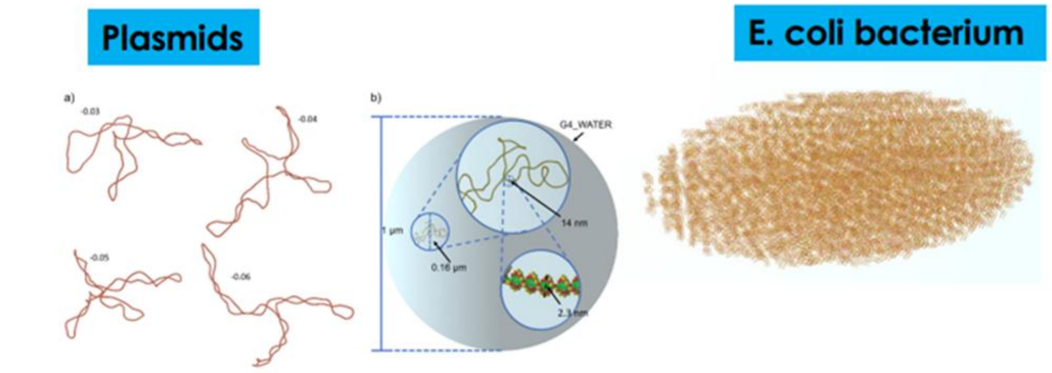
- Pending requirement for many years
  - The 1st implementation with geant4 11.3
- For relativistic annihilation 2- or 3-gamma final state considering NLO QED corrections
  - V.N. Baier, V. S. Fadin, V. A. Khoze, E. A. Kuraev, Physics Reports 78 (1981), 293-393.
  - Affect EM shower shape on level $10^{-3}$
  - Background for experiments on the dark matter search
  - /process/em/lowestTripletEnergy 10 MeV – cut needed for effective sampling
- Creation of ortho (s=1) or para(s=0) positronium at rest concerns mainly medical applications
  - A choice of model for sampling of final state is provided via enumerator
  - G4PositronAtRestModelType
    - fSimplePositronium – current default
    - fAllisonPositronium
    - fOrePowel
    - fOrePowelPolar
    - /process/em/setPositronAtRestModel Allison – variant of selection
    - Allison uses only two gamma Allison model but considers Doppler boarding
    - OrePowell for 2 gamma uses Allison, for 3 gamma - OrePowell model (D. Bernard)
- Quantum entanglement is applied only on 2 first gamma
- Probability of ortho-positronium creation and 3γ decay defined by G4Material property
  - A. Ore and J. L. Powell, Phys. Rev. 75 (1949) 1696
  - R. M. Drisko, Phys. Rev. 102 (1956)1542
  - /material/g4/ortoPositroniumFraction G4WATER 0.05



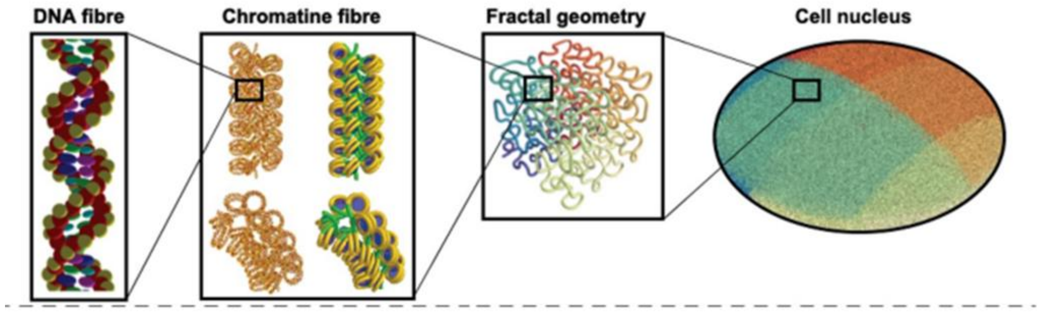



# Medical application and Geant4-DNA

- Medical physics benchmark recently published
  - Includes 23 tests on different aspects of simulation for Geant4 11.2.1
  - Some tests with 11.3 results
- DNA physics and chemistry in Geant4 11.4
  - established combined Physics Lists standard/DNA
  - Standard models above 300 MeV/u for all ions
  - Chemistry code was significantly extended
- Developments for these applications are very useful for HEP
  - Identification of problems in low-energy models
  - Polygon to test technical solution like model combinations per region or per volume



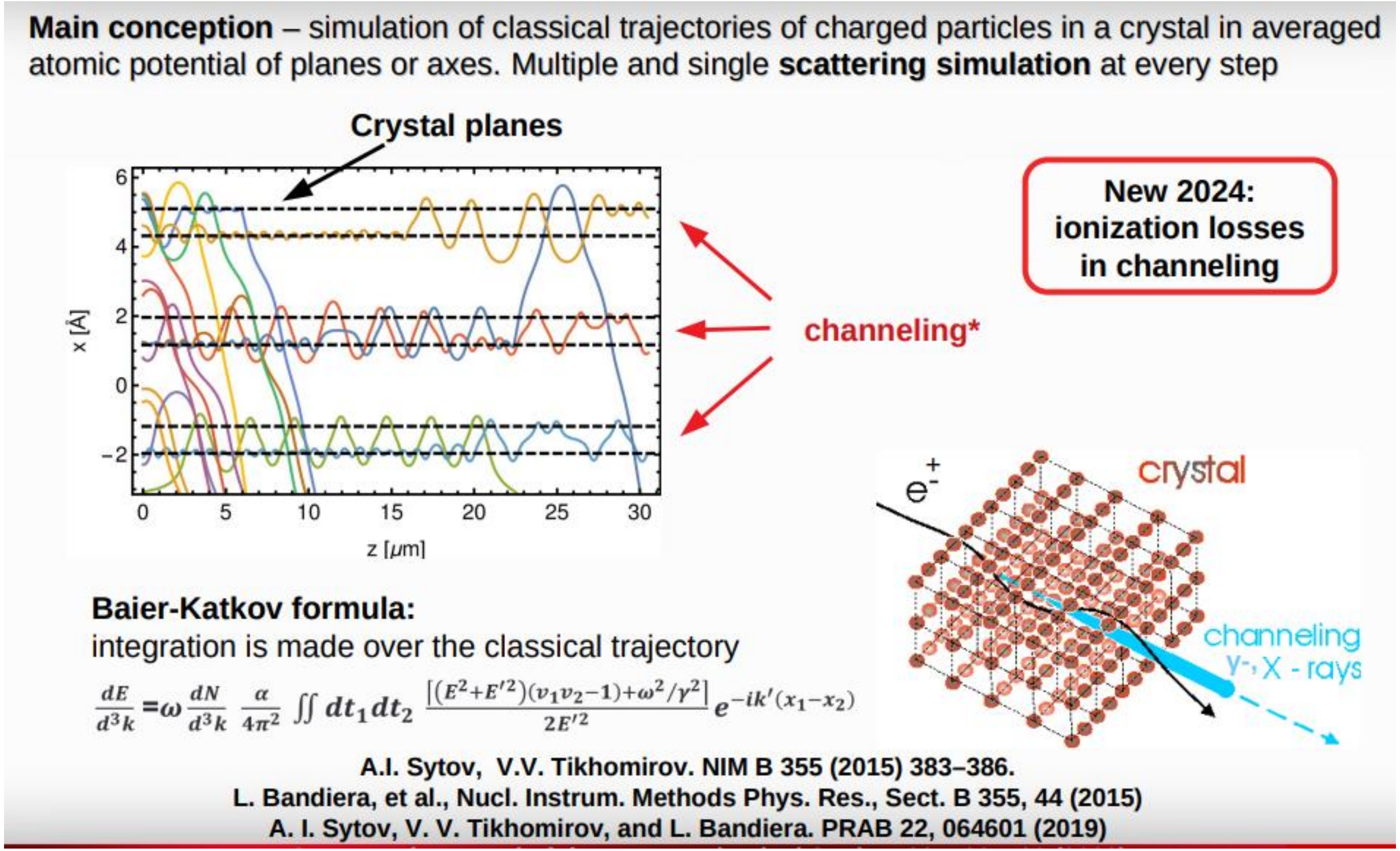

Made available in the “moleculardna” and "dsbandrepair" examples



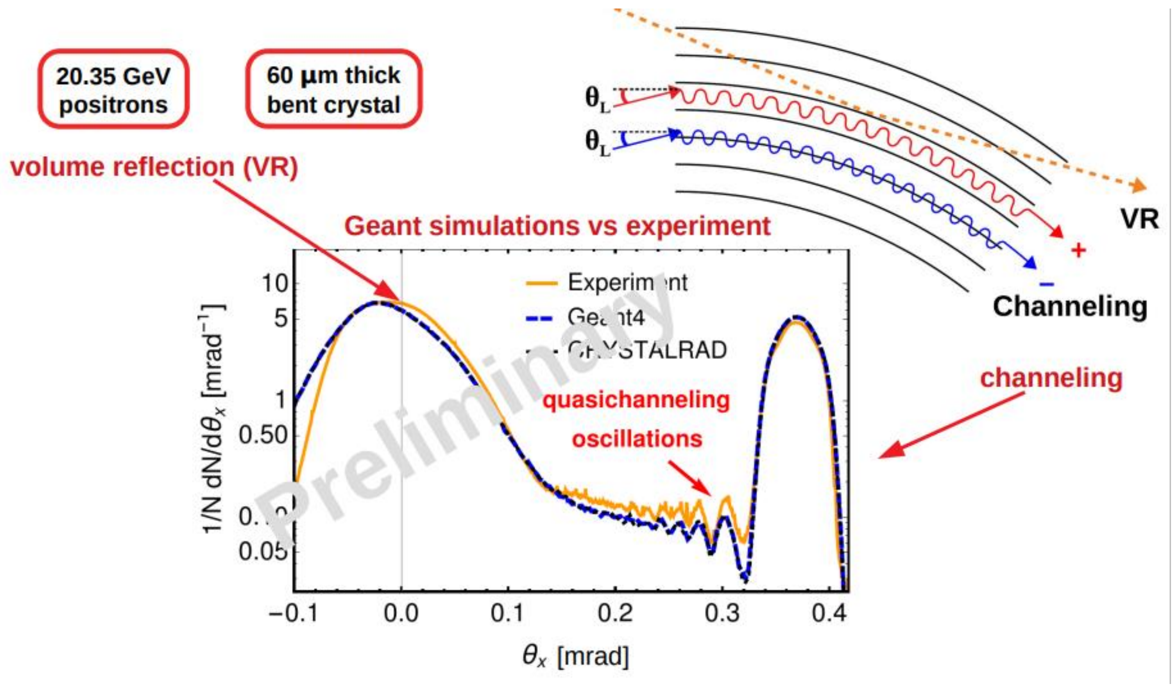

Med. Phys., Special Report, 1–55 (2025)
S. Incerti et al., Medical Physics 37 (2010) 4692–4708
S. Incerti et al., Medical Physics 45 (2018) e722–e739
H. N. Tran et al., Medical Physics 51 (2024) 5873-5889

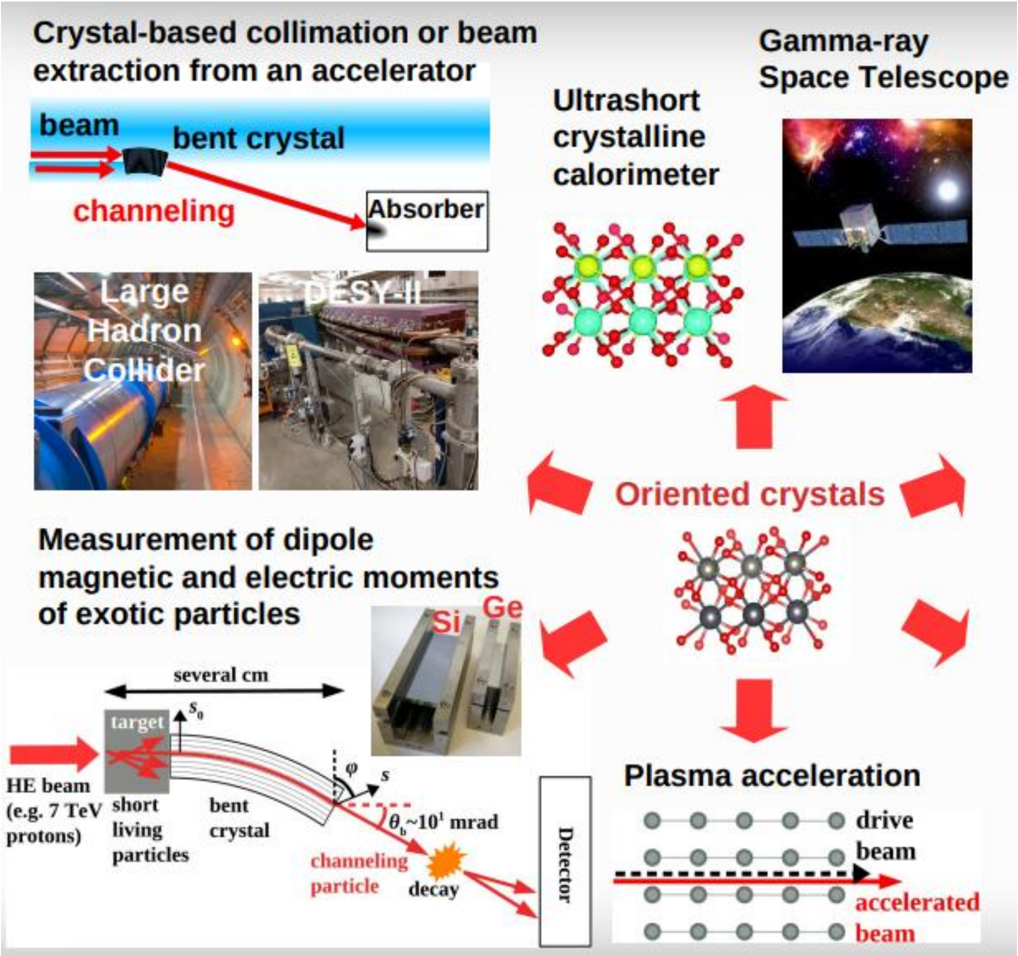
# Simulation of channeling

- Geant4 EM models specialized for oriented crystals
  - These models are applied on Geant4 logical volume
  - Outside there is standard EM physics
- Theory was developed by Baier and Katkov



# Experiments and projects



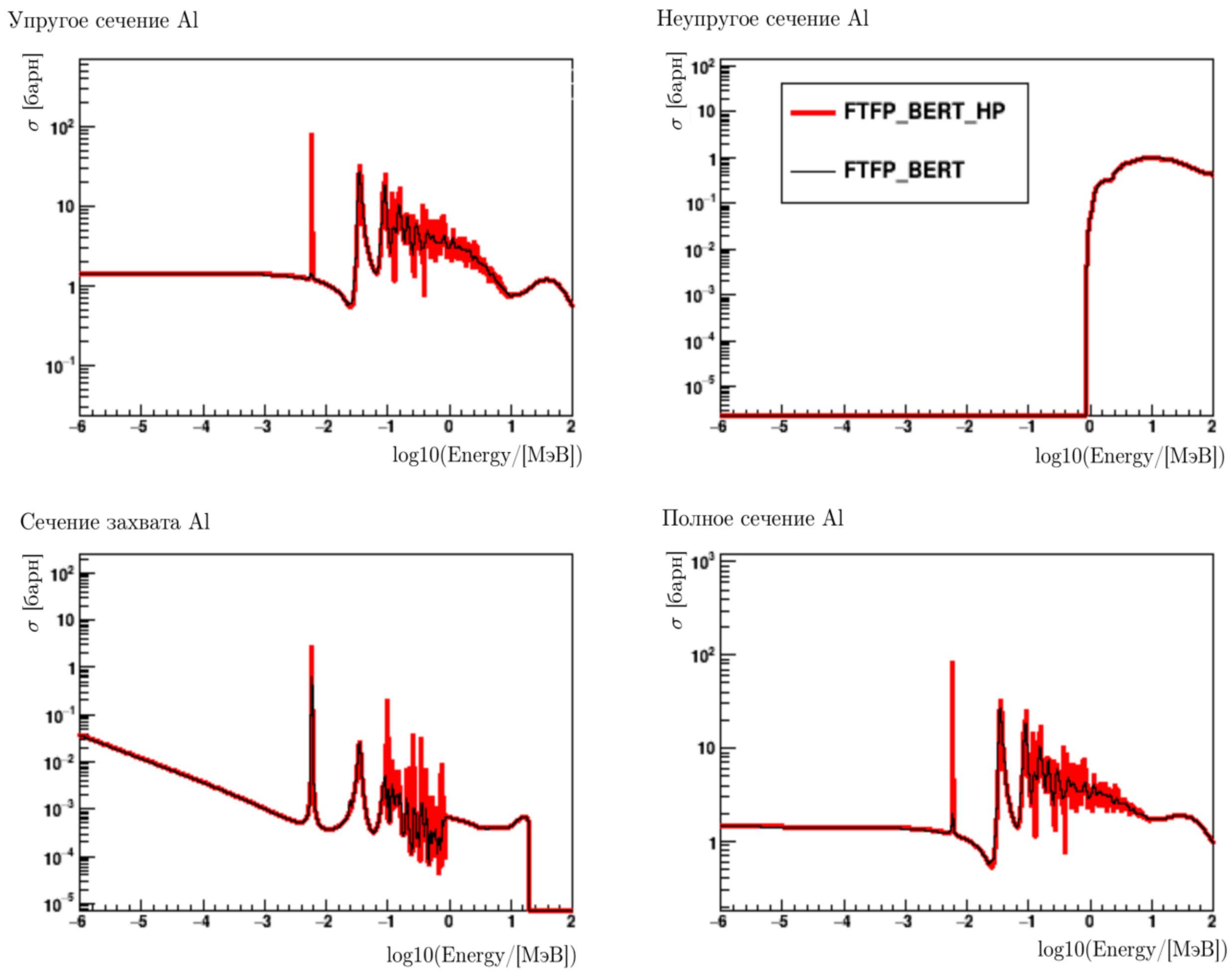

- T. N. Wistisen et al., Phys. Rev. Lett. 119, 024801 (2017)
- A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)
- A. Sytov et al. Journal of the Korean Physical Society 83, 132–139 (2023)

# Hadronic Physics

- Main modifications relevant to LHC experiments were introduced in Geant4 10.5 before Run-3
  - FTF string model and the Bertini cascade
  - Hadronic shower shape in hadronic calorimeters are stable during Run-3
- Hadronic cross sections evaluation are updated
  - The most recent data are used
  - Access methods are optimized
- Since G4 11.2 (2023), interface to Fortran Fluka-CERN available for Geant4
  - Applications to get inelastic cross sections and final states
  - Understood this year some disagreements between Geant4 and Fluka-CERN
    - Due to the different quasi-elastic treatment: considered as inelastic (in Geant4) vs. elastic (in Fluka)
    - Fixed bug in the interface, related to the rotation of final-state particles
  - Under discussion possible extensions (elastic, ion-ion, gamma/lepton-nuclear, …) and C++ version of Fluka
- Light ion QMD model (fully theory based) is introduced
  - relevant to medical applications
- Nuclear de-excitation module is under refinement
  - De-excitation module takes into account  hyper-nuclei
- Low-energy neutron models are updated
  - Thermal neutrons
  - NuDEX code is integrated inside Geant4
- Some selected new developments will be discussed below

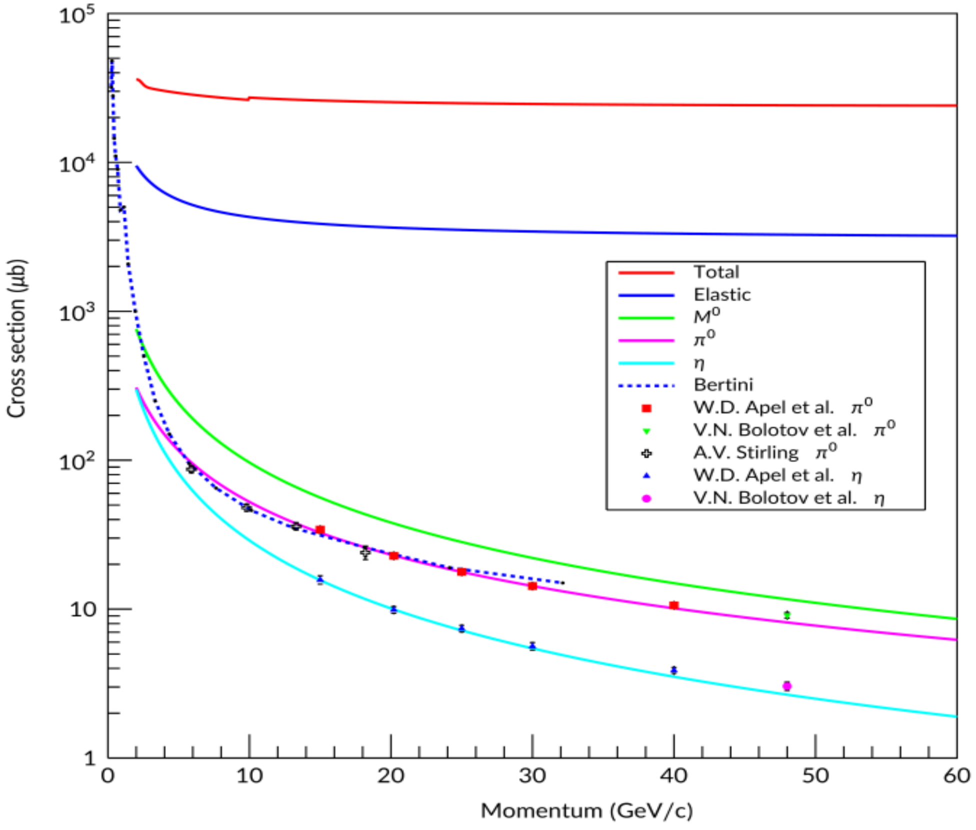
# Hadronic data bases in Geant4 11.3

- Combined approach for cross sections
  - Evaluated data
    - JEFF-3.3, TENDL-2019
    - V.S. Barashenkov cross sections 1989
  - Glauber-Gribov model
    - R. Glauber УФН 103, 642 (1971)
    - V.N. Gribov, JETP 56, 892 (1969)
    - V.M. Grichine, Eur. Phys. J. C 62 399 (2009)
- The new cross sections for neutrons and light ions
  - G4PARTICLEXS4.1
- The new version of data bases for radiative decays and nuclear levels
  - Produced coherently
  - G4ENSDFSTATE3.0
  - PhotonEvaporation6.1
  - RadioactiveDecay6.1.2



# Charge exchange process

- A new Geant4 process for simulation of quasi-elastic charge exchange reactions for pions and kaons
  - $\pi^- + A \rightarrow M^0 + A'$, $M^0 = \pi^0$, $\omega(782)$, $f_2(1270)$ – search on dark matter by NA61
  - $K^- + p \rightarrow K^0 + n$
- The 1st version in Geant4 11.3
  - Significantly improved in Geant4 11.4beta
- Biasing options are available
  - Cross sections may be enhanced



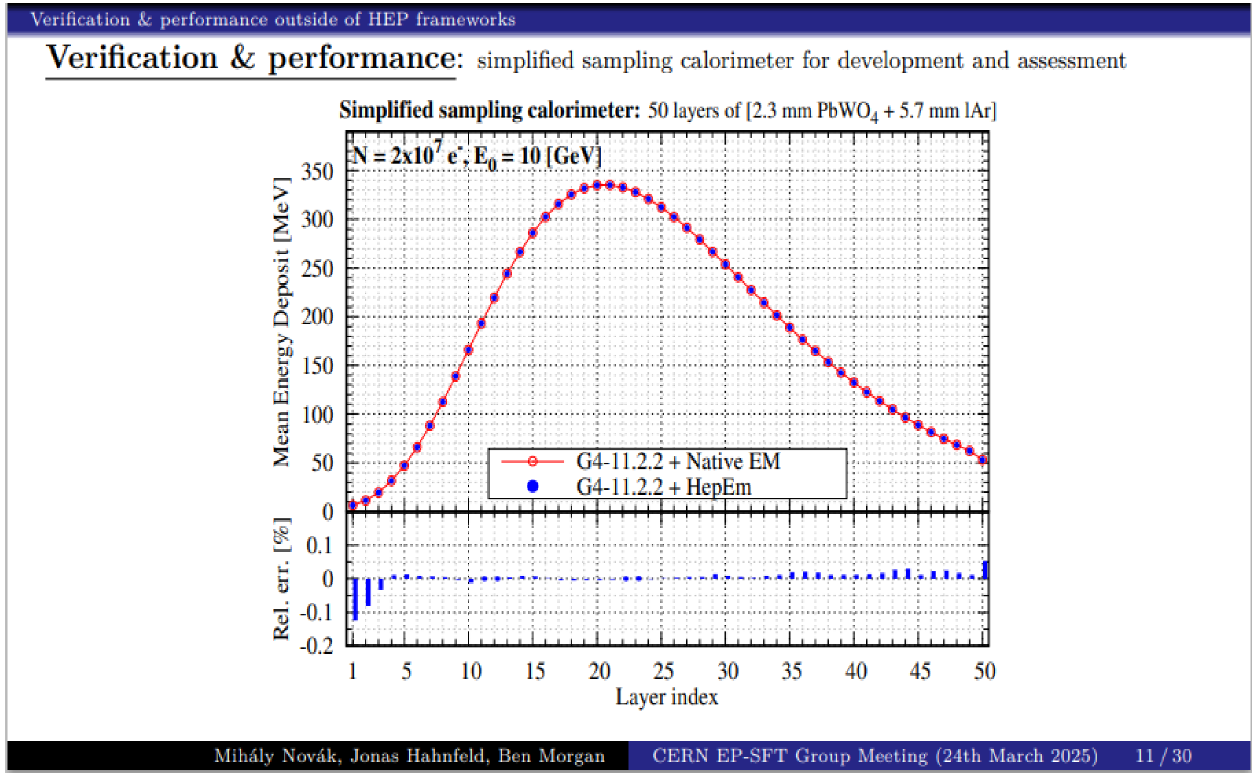
# R&D for Phase2 LHC

- G4HepEm – low energy gamma, e+, e- transport
  - Effective transport at both at CPU and GPU
  - https://geant4-dev.web.cern.ch/collaboration/working_groups/electromagnetic/2024
- AdePT (CERN SFT): https://indico.cern.ch/event/1332507/contributions/5630780/attachments/2771137/4830421/AdePT_evaluation_12_2023.pdf
- Celeritas (ORNL, FNAL, ANL): https://indico.cern.ch/event/1332507/contributions/5630782/attachments/2771072/4828307/rd-review.pdf
- Delta Geant4 assessment of the R&D projects: AdePT and Celeritas, March 26-27, 2025
  - https://indico.cern.ch/event/1507476/
  - Both groups were asked to provide software from specially defined benchmarks and demonstrate results in comparison with the default Geant4 results obtained at CPU

# G4HepEm library to make efficient EM simulation

(M. Novak et al.)

https://indico.cern.ch/event/1518821/contributions/6391131/attachments/3037082/5363687/m_novak_G4HepEm_24_03_2025_sft_meeting.pdf

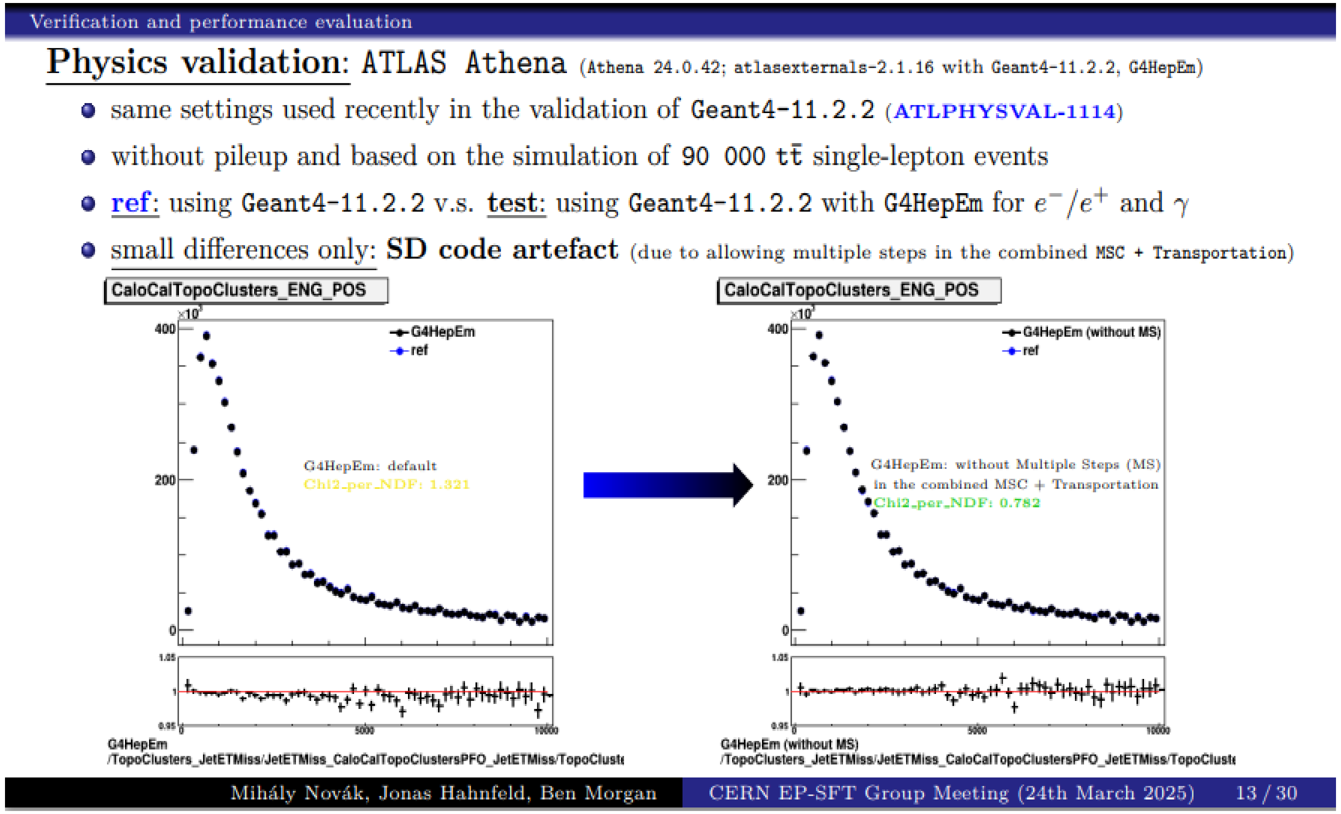


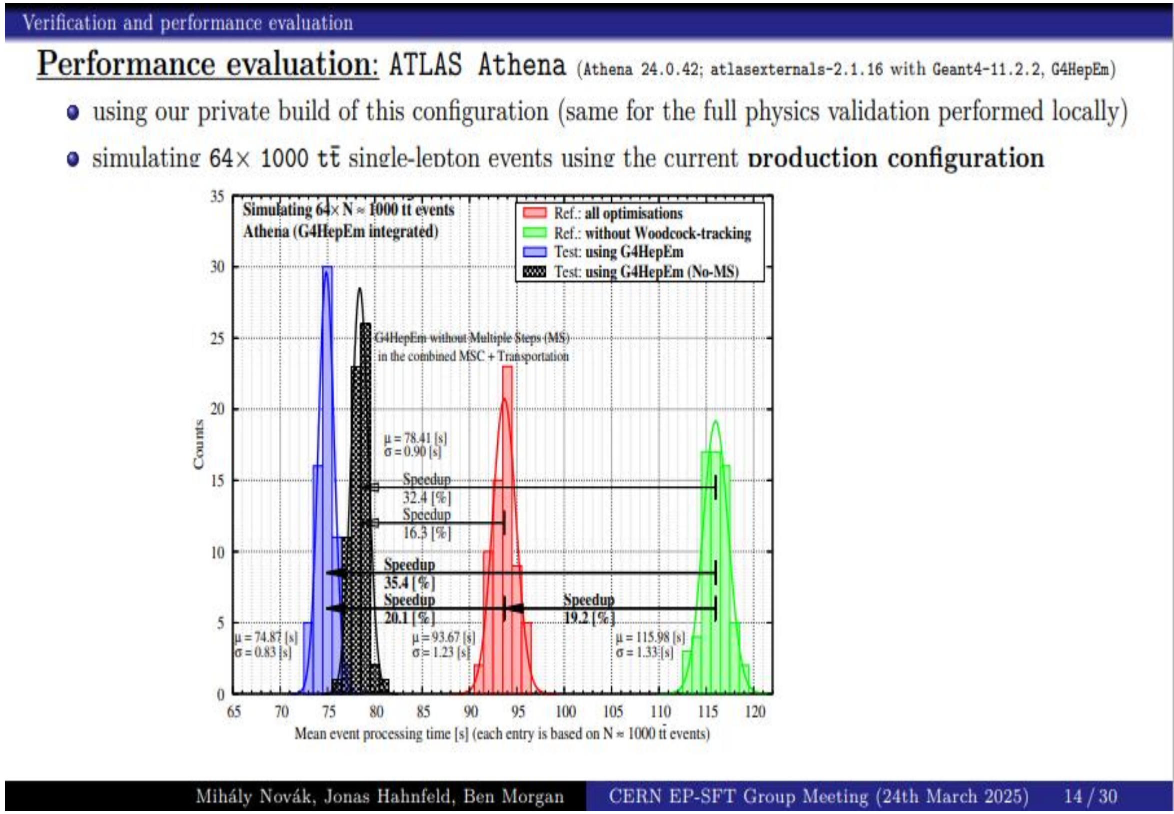

| | | Geant4 EM | HepEm |
|---|---|---|---|
| $E_{dep}$ [MeV] | $PbWO_4$ | 6703.60 | 6708.67 |
| | lAr | 2535.42 | 2531.60 |
| #secondary | $\gamma$ | 4344.51 | 4347.29 |
| | $e^-$ | 1735.31 | 1734.87 |
| | $e^+$ | 425.97 | 426.05 |
| #steps | charged | 26932.3 | 12141.1 |
| | neutral | 40207.9 | 8586.5 |
| Time (60 threads) | | 2272.87 [s] | 1199.25 [s] |
| Speedup | | | 47.27 [%] |

- Simplified sampling calorimeter application

# ATLAS Athena setup (M.Novak et al.)

https://indico.cern.ch/event/1518821/contributions/6391131/attachments/3037082/5363687/m_novak_G4HepEm_24_03_2025_sft_meeting.pdf

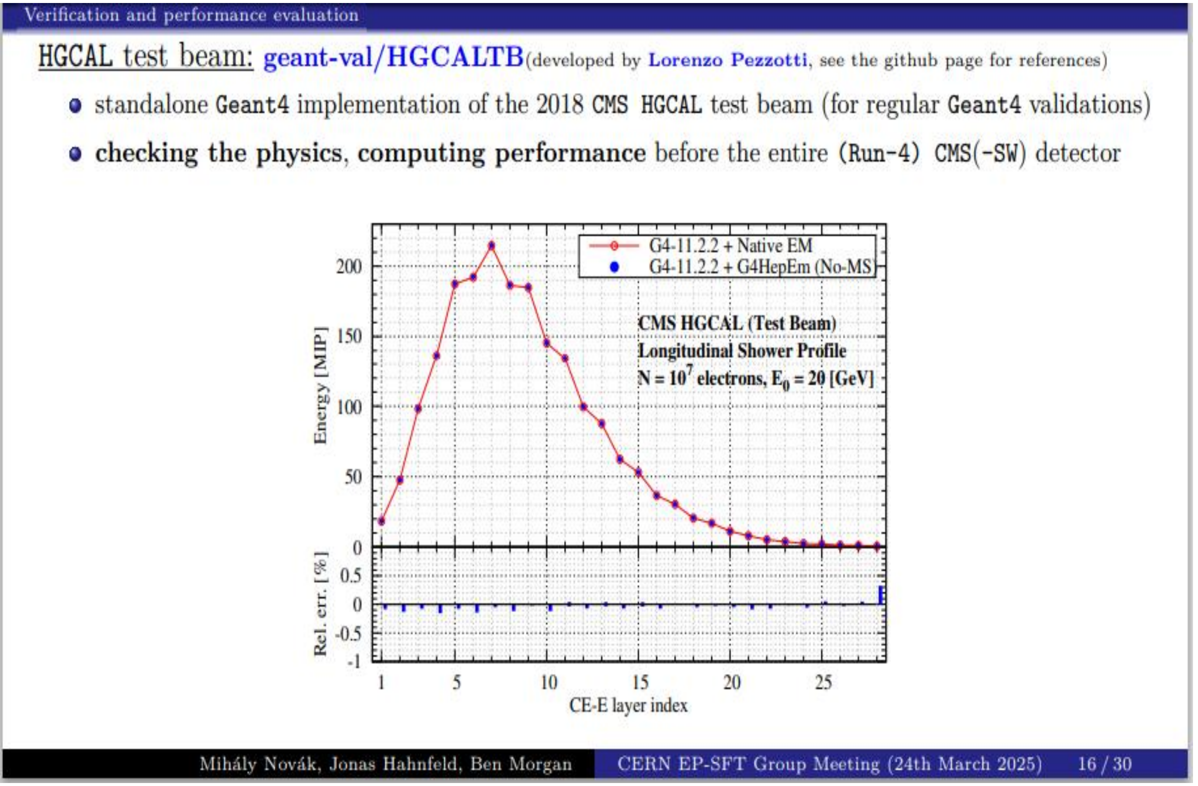



❖ATLAS production speed-up is estimated on level of 20%.

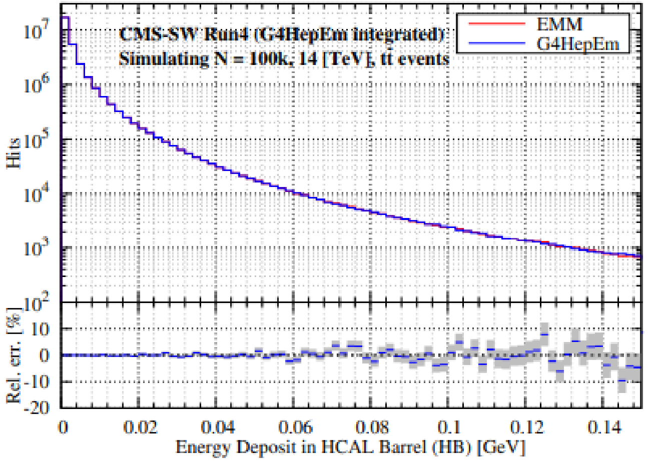
# CMS CMSSW setup (M. Novak et al.)

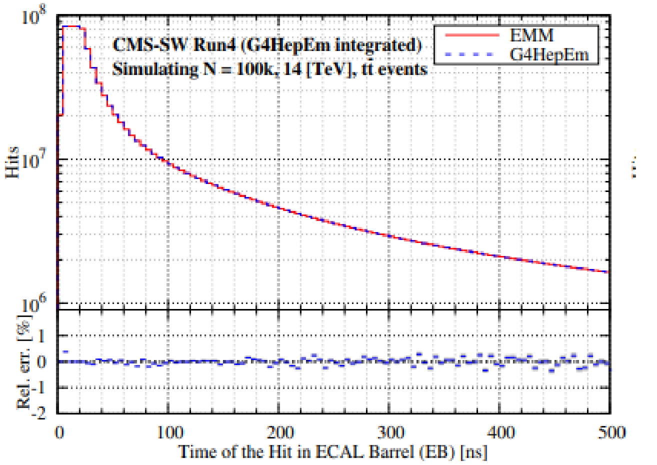
https://indico.cern.ch/event/1518821/contributions/6391131/attachments/3037082/5363687/m_novak_G4HepEm_24_03_2025_sft_meeting.pdf




| $e^-, E = 20[GeV]$ $N = 32\ 000$ | Geant4 Native EM/opt0 | HepEm default | HepEm No-MS |
|---|---|---|---|
| Time (64 threads) | 295.48/312.61 [s] | 148.14 [s] | 154.1 [s] |
| Speedup | | 49.9/52.6 [%] | 47.8/50.7 [%] |

| $\pi^-, E = 20[GeV]$ $N = 32\ 000$ | Geant4 Native EM/opt0 | HepEm default | HepEm No-MS |
|---|---|---|---|
| Time (64 threads) | 116.58/120.2 [s] | 78.78 [s] | 79.86 [s] |
| Speedup | | 32.4/34.5 [%] | 31.5/33.6 [%] |



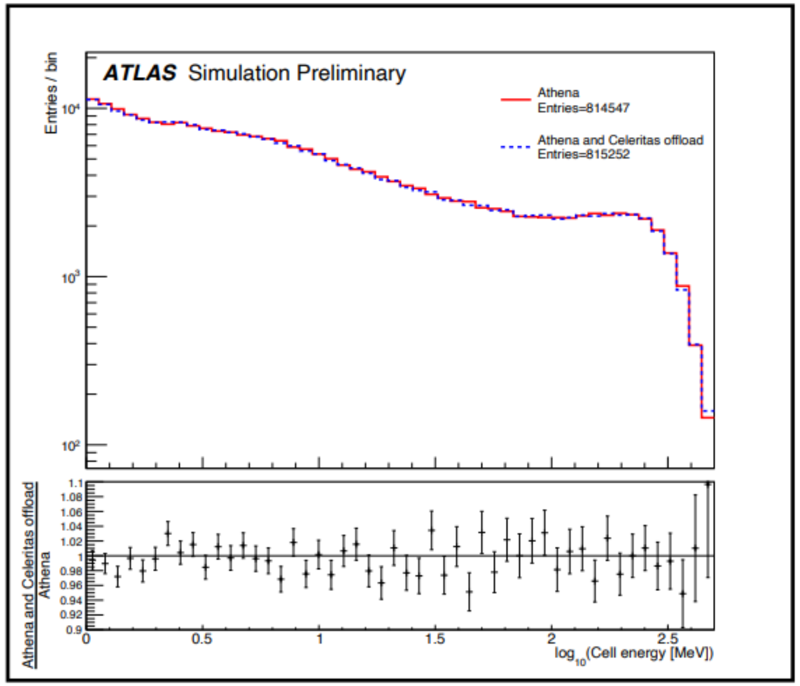




- CMS speedup for ttbar events
  - Run3 – 14%
  - Run4 – 21%

# Celeritas project for GPU (S. R Johnson)

https://indico.cern.ch/event/1507476/contributions/6343926/attachments/3039428/5368372/celeritas-overview.pdf

- Current status after 5 years R&D
- Celeritas physics is equivalent to EM standard physics of Geant4
  - No $\gamma$, electro-nuclear
  - selectable processes and physics options
- Full-featured Geant4 detector geometries using VecGeom
  - Both solid and surface models
  - arbitrary field definition
- Considered extensions
  - Neutron transport
  - Optical photons transport

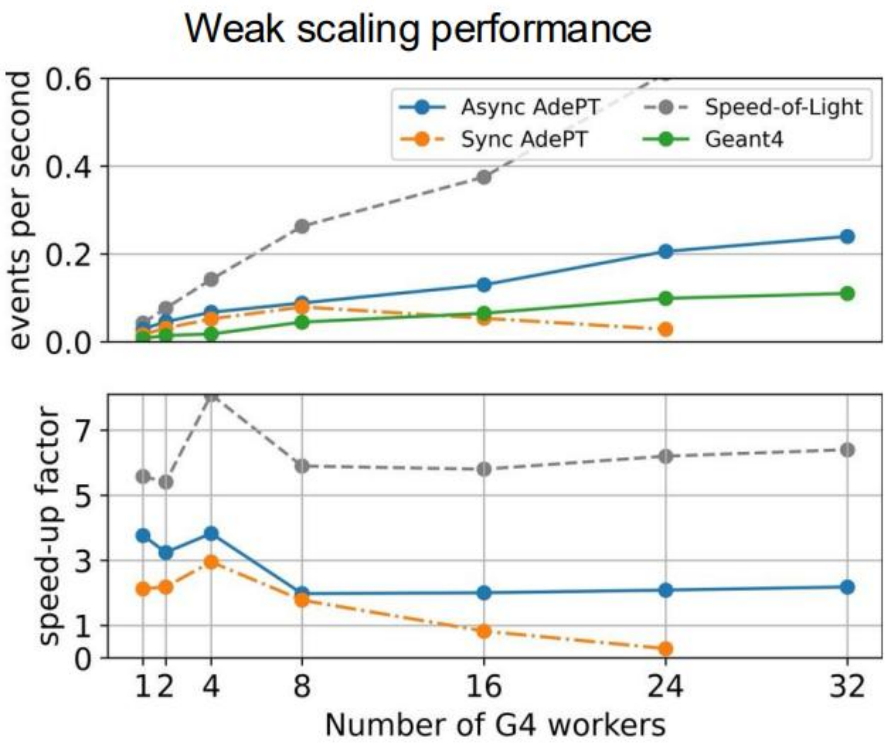



**Cell energy distribution** in TileCal; red: CPU-only Geant4, blue: GPU-accelerated e±/γ with Celeritas

# Geant4 simulation at GPU with AdePT

https://indico.cern.ch/event/1507476/

- G4HepEm physics
  - Gamma, electro-nuclear physics are identified, and track returned to sample interactions at CPU
  - Only baseline EM models are included into this sub-library
- VecGeom geometry
  - Converted from Geant4 native geometry, may use surface model
- Magnetic field based on 3D field map
  - ACTS project from ATLAS using Runge-Kutta propagator
  - DormandPrince45 field integrator used for CMS
- Asynchronous mode is required to achieve improved CPU performance
  - Tracks are propagated in the setup in parallel
  - MC truth handling in the experiment software should be changed
    - Current Geant4 software assumes continues treatment of tracks



# Requirements to GPU code for HEP

- Usage of GPU should speed-up simulation
  - Maximum theoretical factor 3 if only $\gamma$,e+- physics is at GPU
  - Speed-up factor > 1 is a minimal request
  - Asynchronous mode is needed to be efficient
- CPU and CPU+GPU modes should provide the same physics
  - Minimal requirement $10^{-3}$ statistical agreement for high statistics experiments
    - Geometry and tracking in field
    - Physics should be the same
  - Reproducibility should be provided
    - Coherent handling of random numbers
- Notes:
  - CPU mode in any case will provide an opportunity to use alternative models and high order corrections to existing models
  - Hadronic physics in general not easy (or impossible at GPU)
  - In case of success of R&D the MC truth software of experiments should be re-written

# What is expected in 2025?

- Geant4 work plan includes many items
  - https://geant4-dev.web.cern.ch/news/2025-03-11-planned-dev
- Important for HEP users
  - Parallel initialization of geometry and physics
  - Fluctuations of energy loss per G4Region
  - Cerenkov and Scintillation processes configurable per logical volume
  - Updated cross section data sets
  - Updated Bertini cascade
  - Updated nuclear de-excitation module
- R&D projects
  - Expected AdePT and Celeritas adaptation for experiment frameworks
    - Work is ongoing in ATLAS, CMS, LHCb

# Conclusions

- Geant4 is a long-term project
  - It cannot be in “done” state, because new requirements appear
  - The team is trying to keep stability and progress at the same time
- Progress includes new technical features
  - New compilers, improved C++ patterns
- New advanced models are integrated into the toolkit
  - More external libraries are used now
    - G4HepEm, AdePT, Celeritas, PHYTHIA, Fluka
  - Advanced physics models for low- and high-energy applications
  - Cross sections and data bases are updated as well
  - The Geant4 Collaboration is open for new ides and models from users

# Thank you for attention