Geant4 in the ATLAS experiment

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Geant4 Technical Forum
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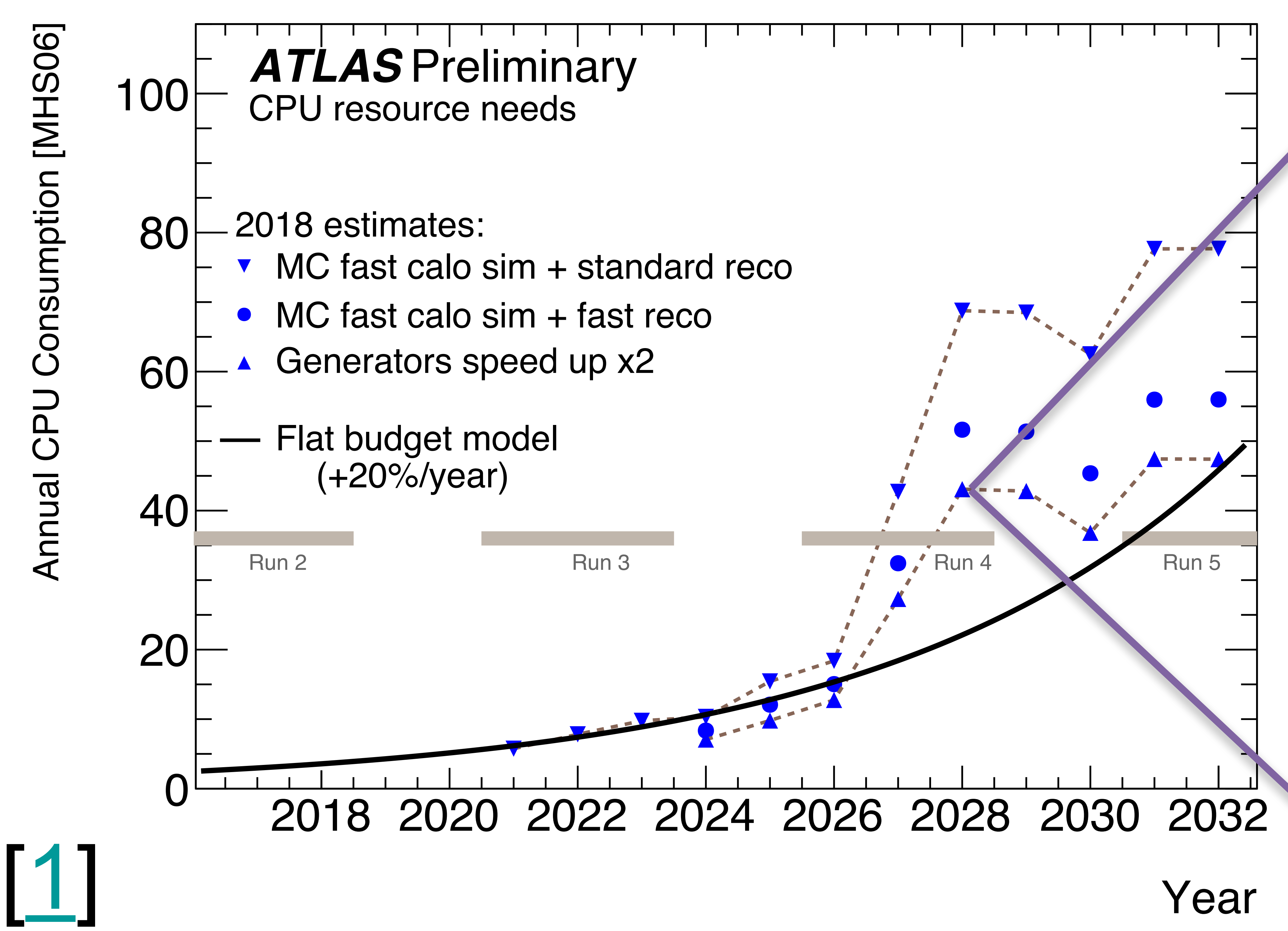
- In Run 3 and beyond, the majority of events will be processed with fast simulations, however, Geant4 simulation is expected to remain the main CPU consumer in ATLAS even in Run 4,
- Software improvements in Geant4 simulation are necessary in order to keep up with the increasing luminosity and the evolving hardware,
- Speeding-up our simulation will allow for the production of more MC statistics and reduce the statistical uncertainty that many analyses face.



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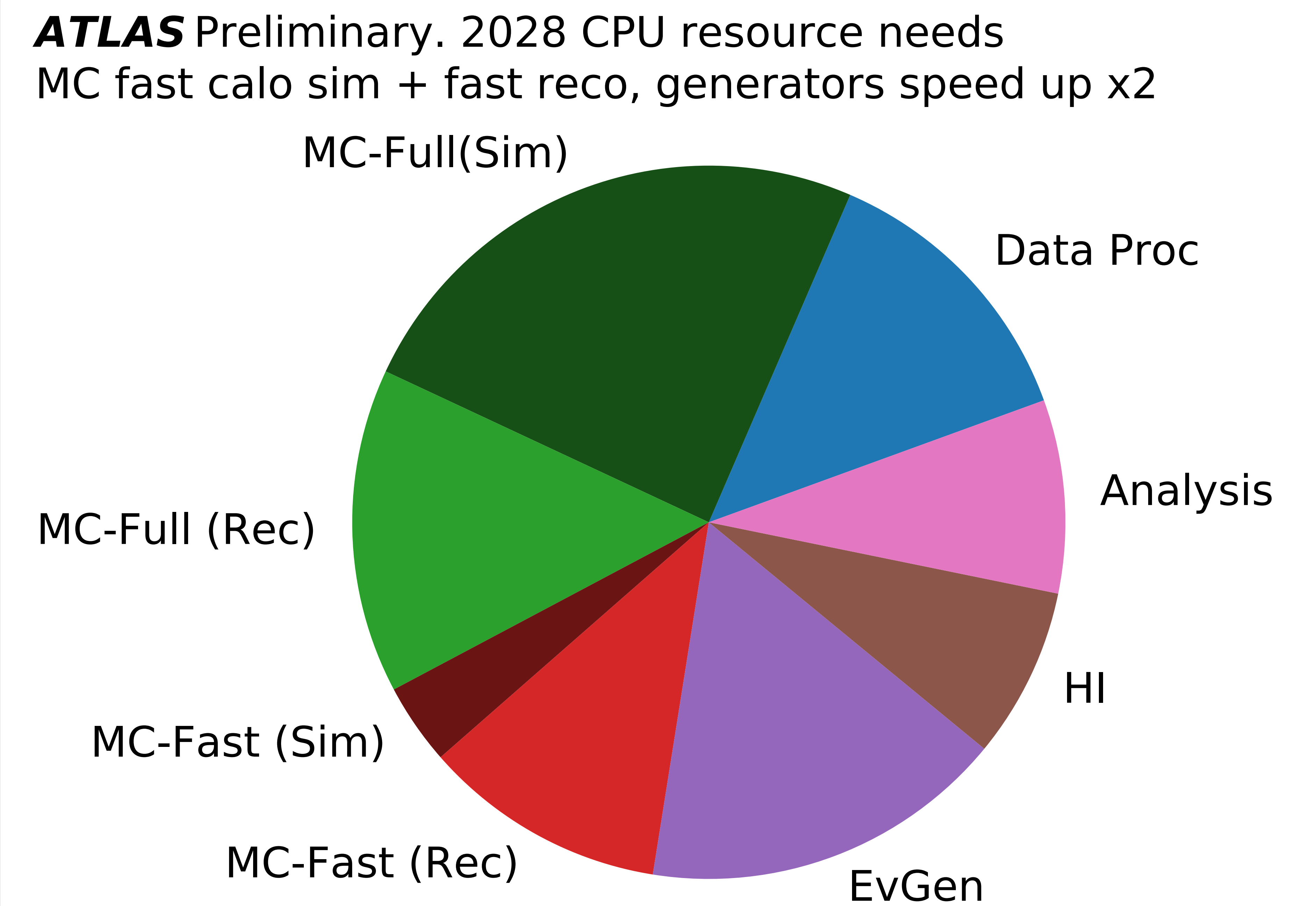

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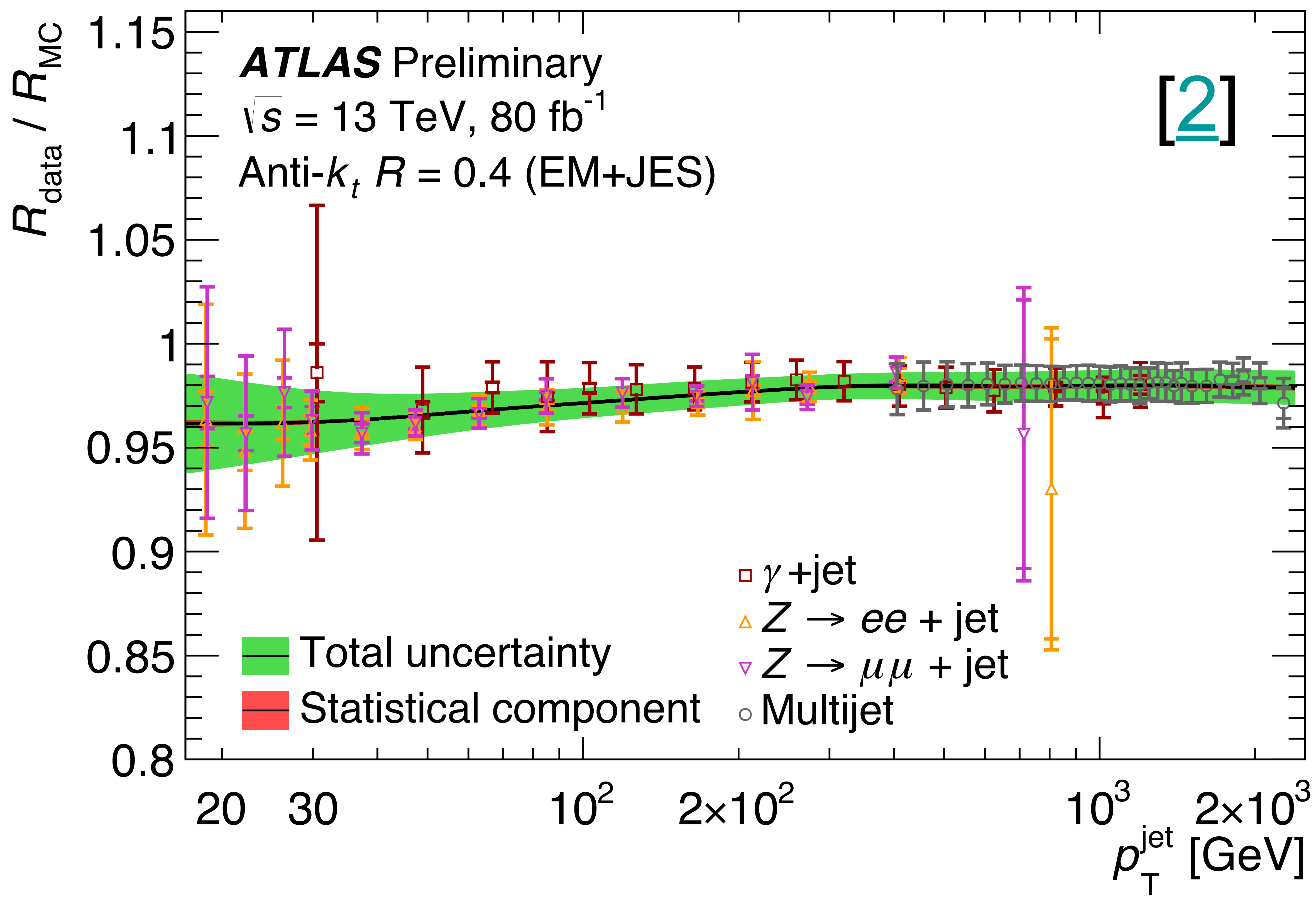
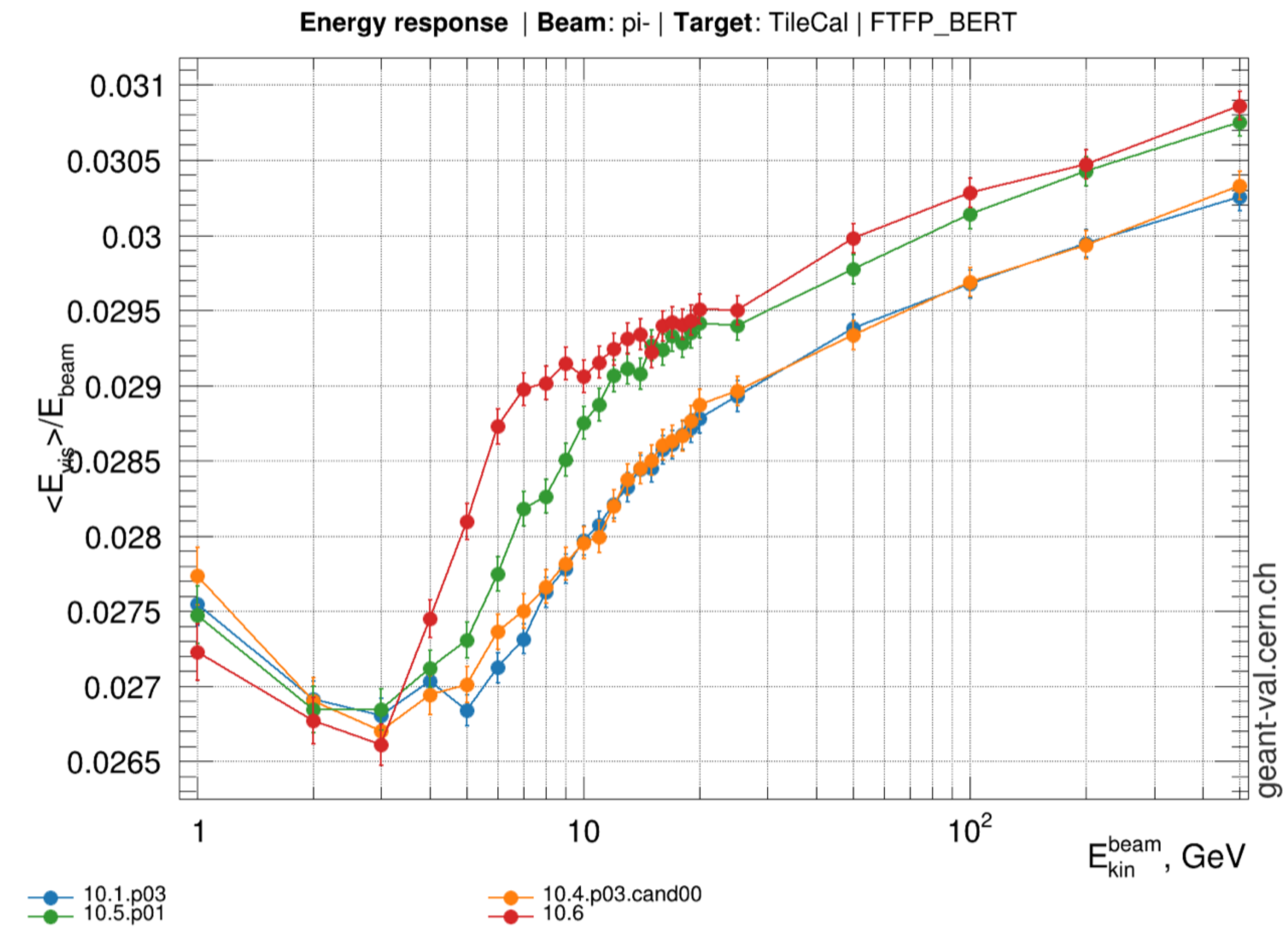
Introduction Cont'd

- Follow up on Marilena's detailed report in January: https://indico.cern.ch/event/872309/contributions/3701721/attachments/1970909/3278381/Atlas_update_MarilenaBandieramonte.pdf
- Developments since January:
  - Firsts tests with Geant4 10.6,
  - Further and more stringent physics validation tests for Neutron Russian roulette and EM range cuts,
  - Refined MT scaling studies,
  - Ongoing work on MT migration, geometry optimization, quasi-stable particle simulation.

- ATLAS has been using Geant4 10.1.3 for Run 1 and Run 2 and we are planning to move to a newer version for Run 3,
- ATLAS MC continues to have a 3-4% higher response than the data for jets,
- Updates in hadronic physics in newer versions are expected increase the response even further —> problem for ATLAS.





Strategy for deploying new Geant4 versions

- Plan to adjust Birks’ constant to compensate for larger energy response,
- Test different values of Birks’ constant in HEC and Tile test beam data,
  - Vary Birks' constant → recalculate sampling fractions → compare ratio of EM/hadronic response to data.

- Plan to test three Geant4 versions: 10.1.3, 10.4.3, 10.5, 10.6,
  - Compiled ATLAS simulation infrastructure with all versions, but had some issues transitioning to G4IntegrationDriver from G4MagInt_Driver.

- In addition, plan to test different G4Steppers and G4InterpolationDriver (ATLAS currently using G4NystromRK4),
  - E.g. would like to test G4DormandPrince with G4InterpolationDriver.

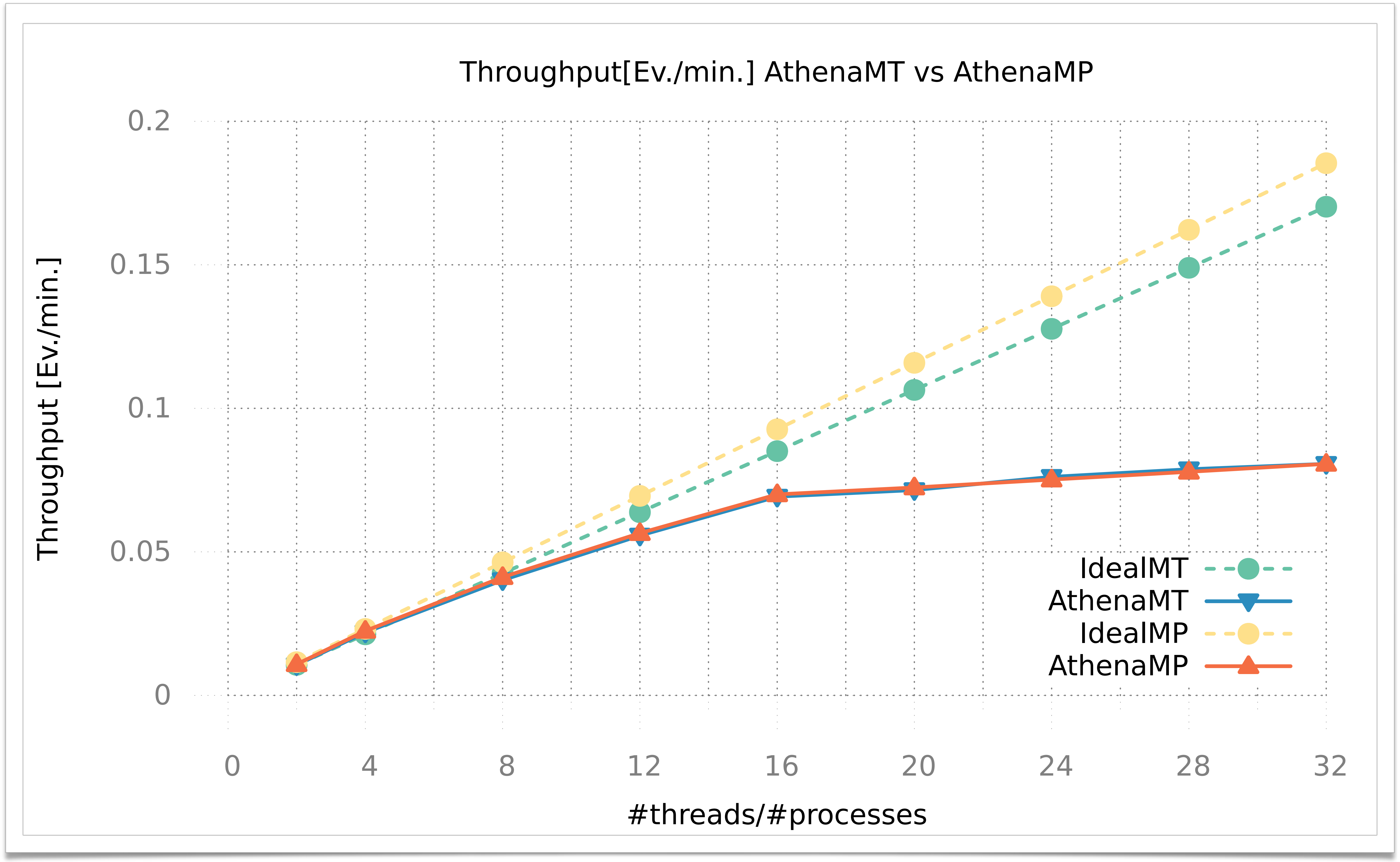
G4IntegrationDriver vs G4MagInt_Driver

- In 10.1.3, ATLAS has been using G4MagInt_Driver where the stepper is referenced as G4MagIntegratorStepper,
  - In this scheme all stepper calls are virtual,
- In newer versions, this was reimplemented with G4IntegrationDriver<*StepperType*> where stepper is templated,
  - Virtualization moved one layer up to improve performance.

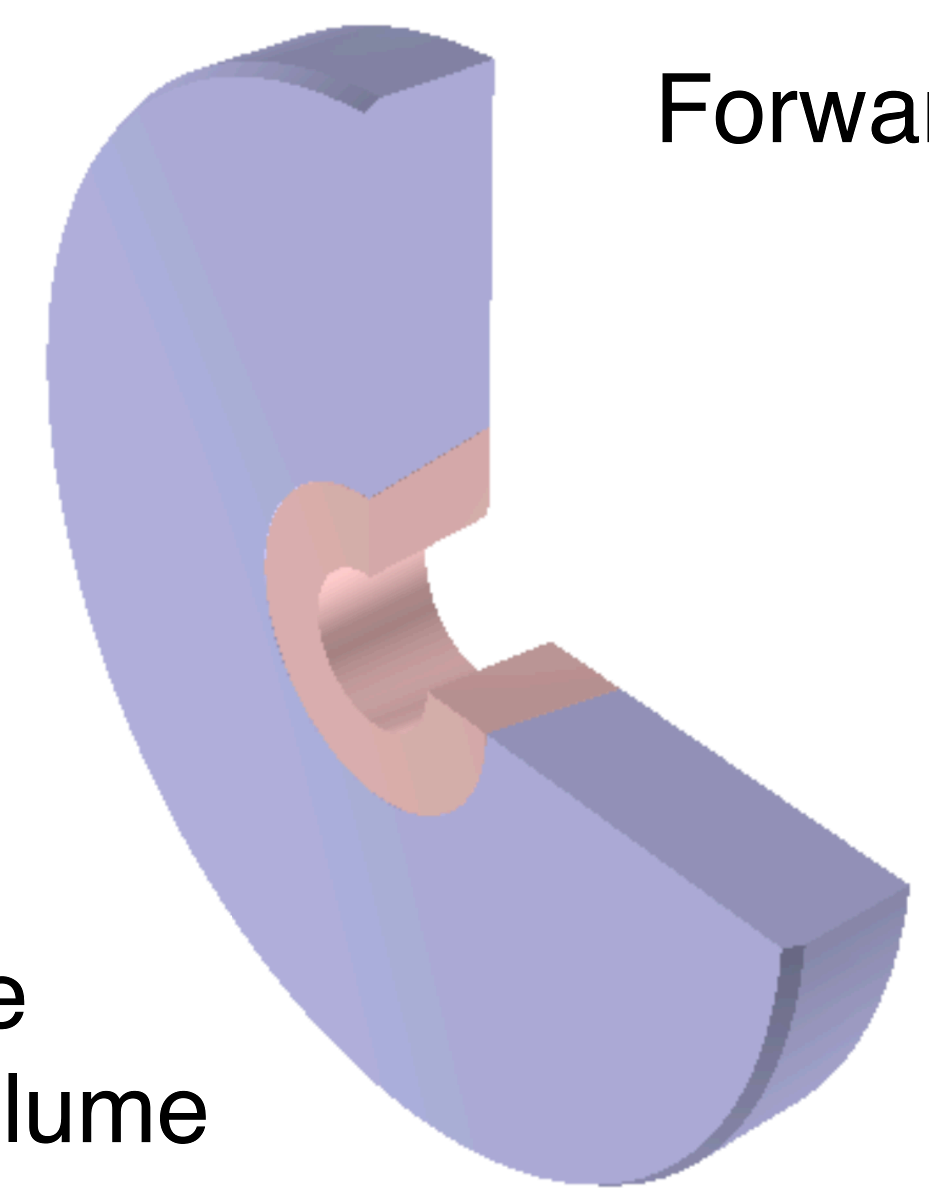
- However, in ATLAS we spotted that output of simulation changes when using G4IntegrationDriver instead of G4MagInt_Driver,
  - Difference present in 10.4.3 and newer versions (did not test any older),
- With great help from John Apostolakis we pinpointed some minor differences in the implementation and are currently testing reproducibility,
  - e.g.: the number of iterations is counted / checked badly in G4MagInt_Driver and exceeded the maximum by two.

Geant4 MT

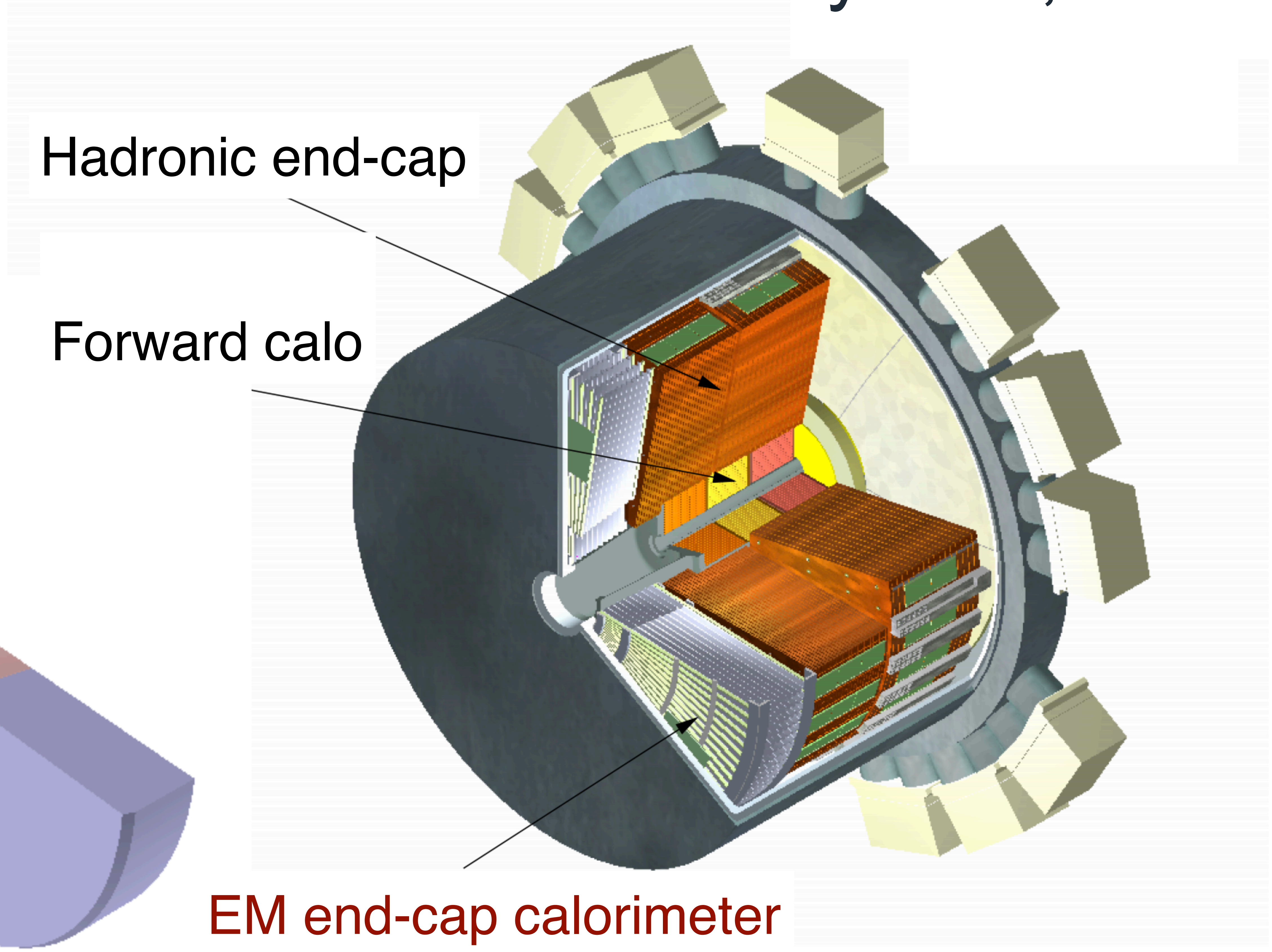
- Large-scale (100k events) tests with stand-alone (no ISF) ATLAS Geant4 successful in MT and physics validation shows no issues,
- Same CPU scaling as with the 'MP' approach and greatly improved memory usage,
- Working on testing Geant4MT running as part of ISF (Integrated Simulation Framework) which will be the production default,
  - Currently runs with multiple threads and gives consistent results,
  - Some parts still need to be migrated (e.g. Frozen Showers),
  - Physics validation needed.
- For more details see [Marilena's talk in January]() or [Marilena's CHEP talk]().



- A speed-up of about 4% was found to be possible with VecGeom in ATLAS with Geant4 10.4,
- This is mostly limited by the EM end-cap volume, which is a custom solid and is therefore unaffected by VecGeom,
- G4Solids account only for about 10% of total simulation time in ATLAS, and a majority is contributed by G4Polycone objects which are notoriously slow,
- A G4Polycone is used for the bounding volume of the EM end-cap,
- Few percent additional speed-up can be achieved by a more efficient bounding volume description of the EM end-cap.

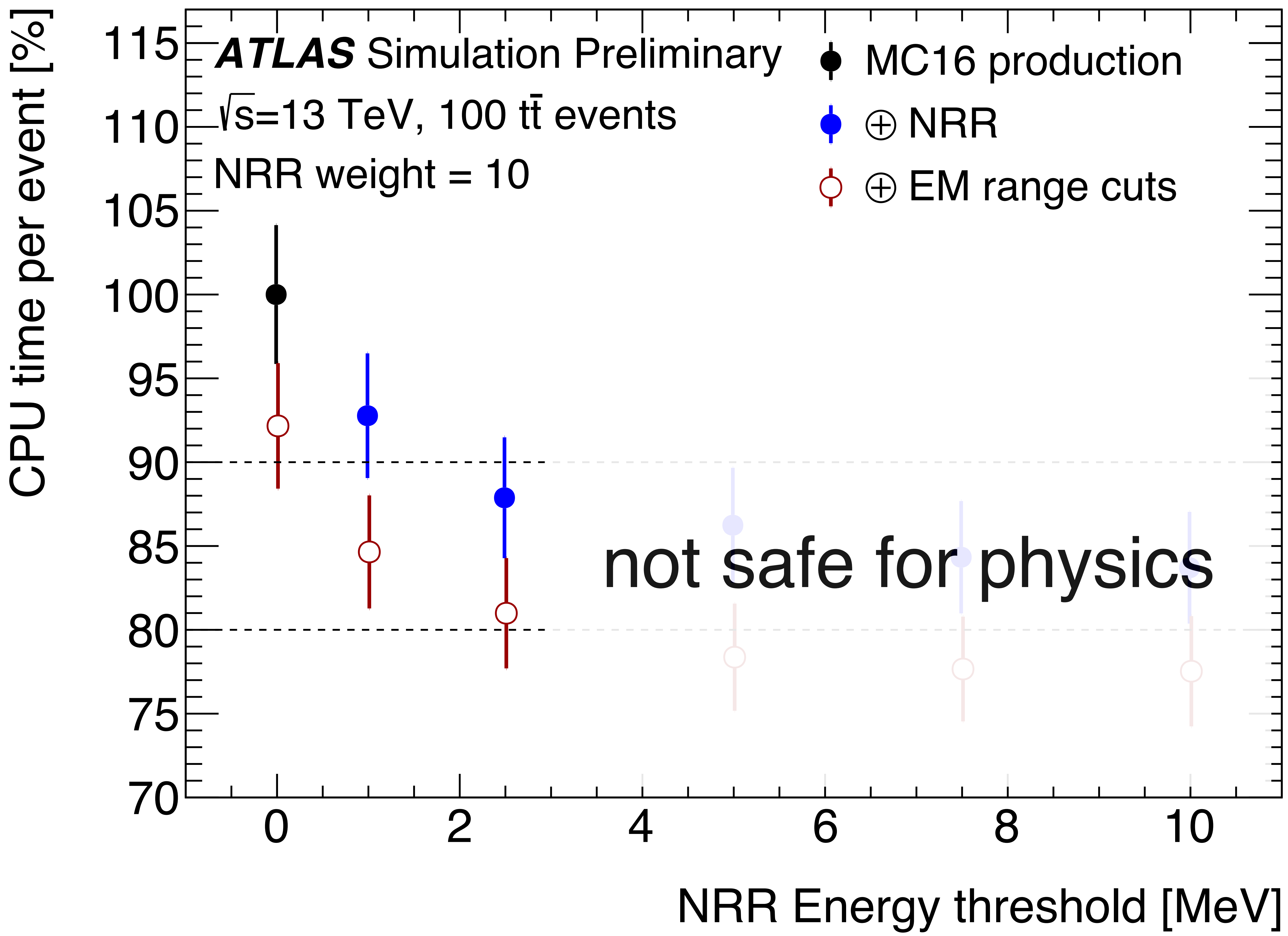


G4Polycone used to describe
the EM end-cap bounding volume



Geant4 performance optimizations

- Neutron Russian Roulette (NRR) with E_{th} = 2 MeV and w = 10 and range cuts for EM processes (compton, photo-electric, conversion) adopted for next round of simulation,
- Other improvements under investigation: Photon Russian Roulette, 'large static library', further geometry optimizations,



- Geometry optimizations, NRR, and range-cuts already bring a 20% speed-up compared to the Run 2 production setup,
- Additional speed-up is expected to be achieved for Run 3 production,
- Might need re-optimization with Geant4 version change.
- More info: Miha's CHEP talk.

Quasi-stable particle simulation

- Quasi-stable particle: ‘a particle which propagates outside the beam-pipe, but has already been decayed by the generator’,
- Geant4 will propagate quasi-stable particles for lifetime from the Generator applying bending in the magnetic field and EM physics such as energy losses due to ionization,
- Once the lifetime is reached Geant4 decays the quasi-stable particle according to its pre-defined decay,

- ATLAS developments:
  - Special treatment needed for particles with zero life-time (e.g. B-meson oscillations) which are not handled well by Geant4 (see backup),
  - Added particles unknown to Geant4 using the PDF table to enable some of the decays e.g. ($B \rightarrow D^{*}\ldots$).

Summary

- First tests of Geant4 10.6 are underway,
  - Spotted an issue with G4MagInt_Driver having a slightly different implementation than G4IntegrationDriver (already present in 10.4),
- Planning to adjust Birks' constant and use a newer Geant4 version for Run 3,
  - Need to analyze test beam data with different values of Birks' constant and recalculate sampling fractions,
  - Requires stringent physics validation tests with involvement from all physics performance groups and multiple iterations.

- Good progress on MT migration: can successfully run large scale-samples, desired scaling achieved (no loss in CPU, improvement in MEM),
- Adapted Neutron Russian Roulette (E=2 MeV, w=10) and EM Range Cuts which improve CPU performance by ~20% for next round of simulation,
- Photon Russian Roulette, VecGeom, geometry improvements under investigation.

BACKUP

Speed-ups already in place

- For Run 2 MC production ATLAS already used shower libraries in the forward calorimeter and other smaller optimizations to gain performance,
- Relative time compared to the nominal configuration shown in the table below.

Configuration (Geant4 10.1.3)	MinBias	ttbar
Nominal production configuration: shower libraries in the forward calorimeter, nominal range cuts, NystromRK4 stepper, FTFP_BERT_ATL physics list, 250ns neutron time cut, simulation of primary particles with pseudo-rapidity below 6.0	1.0	1.0
No shower libraries	1.5	1.3
ClassicalRK4 stepper instead of NystromRK4	1.09	1.07
No neutron time cut	1.02	1.01
FTFP_BERT instead of FTFP_BERT_ATL physics list	No change	No change

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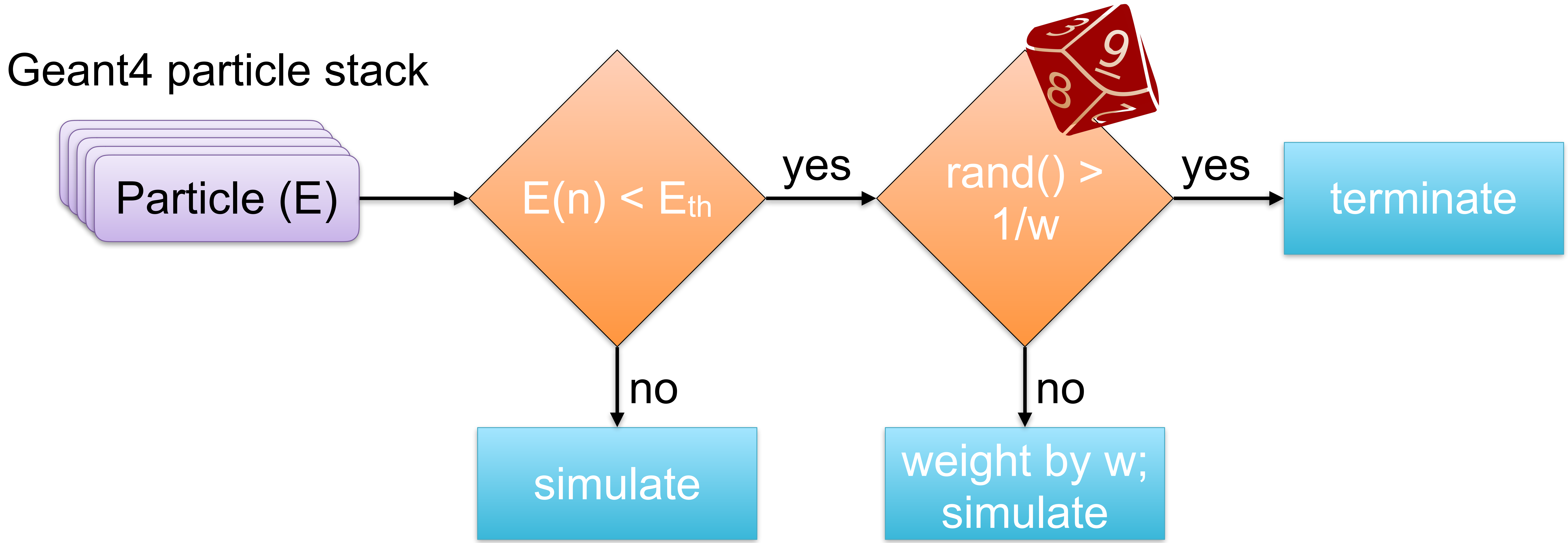
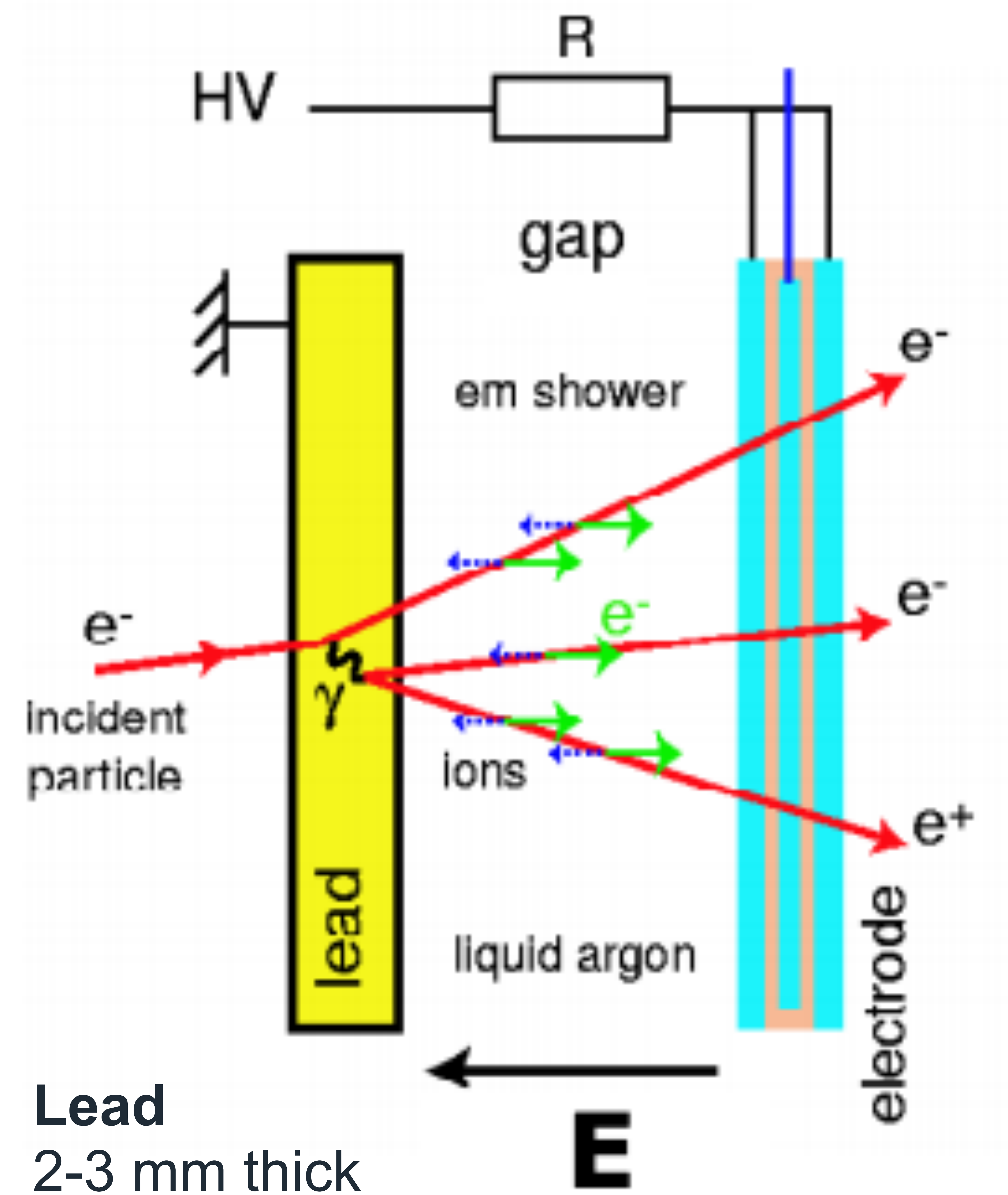
- Randomly discard particles below some energy and weight the energy deposits of remaining particles accordingly:
  - **Energy Threshold** (E_{th}),
  - **Weight** (w): particles below E_{th} are discarded with P((w-1)/w) and energy deposits of remaining particles (and their secondaries) are multiplied by w.



Range cuts

- Range cuts are a built-in way of optimizing Ge
- For each material-volume pair, range cuts can (*mm*),
- Secondaries, that are expected to travel less tl created and their energy is immediately depos
- Most Geant4 processes except processes witl electrons respect range cuts by default,
- ‘compton’, ‘photo-electric’, and ‘conversion’ igr to be activated.



Lead
2-3 mm thick
100 µm range cut

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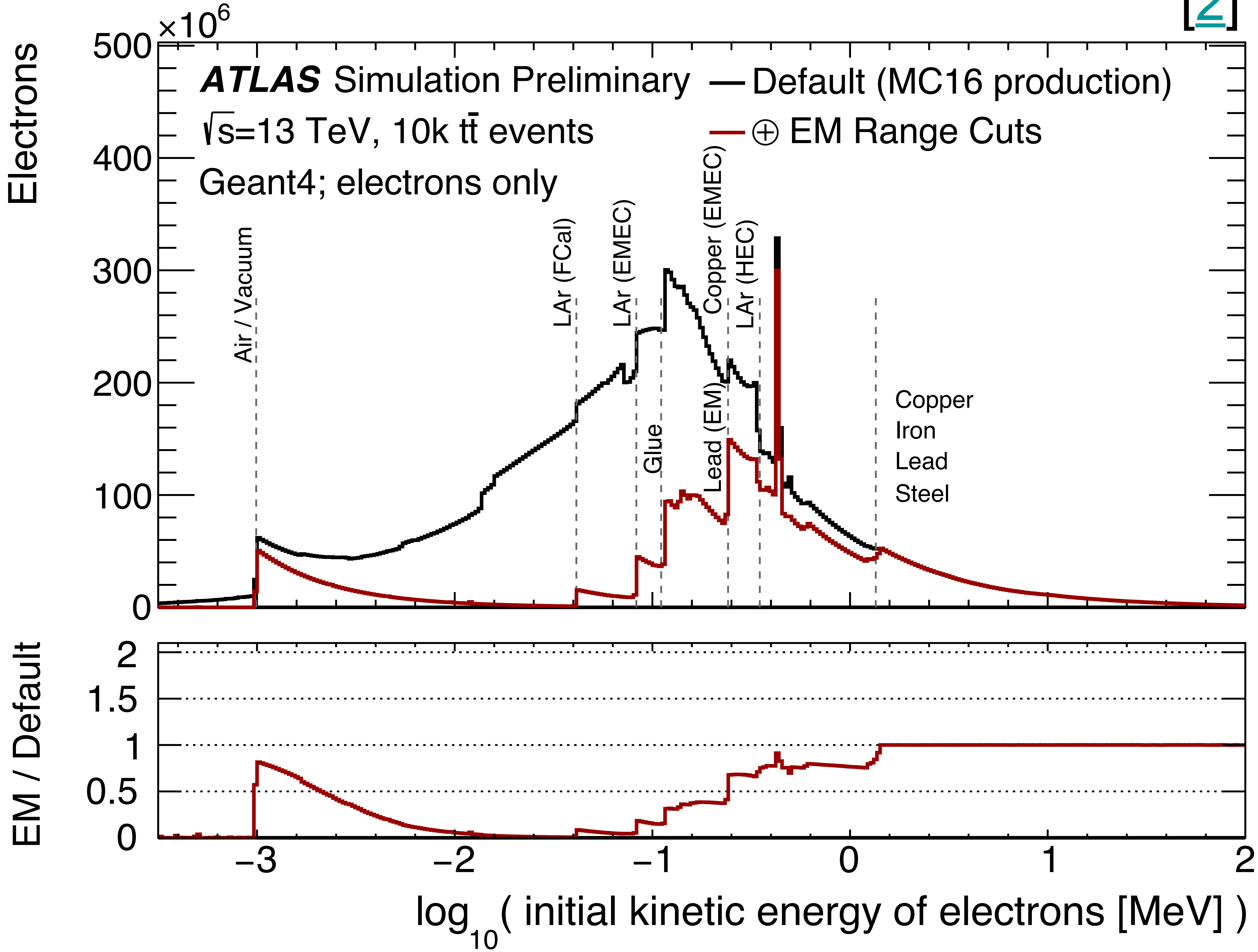
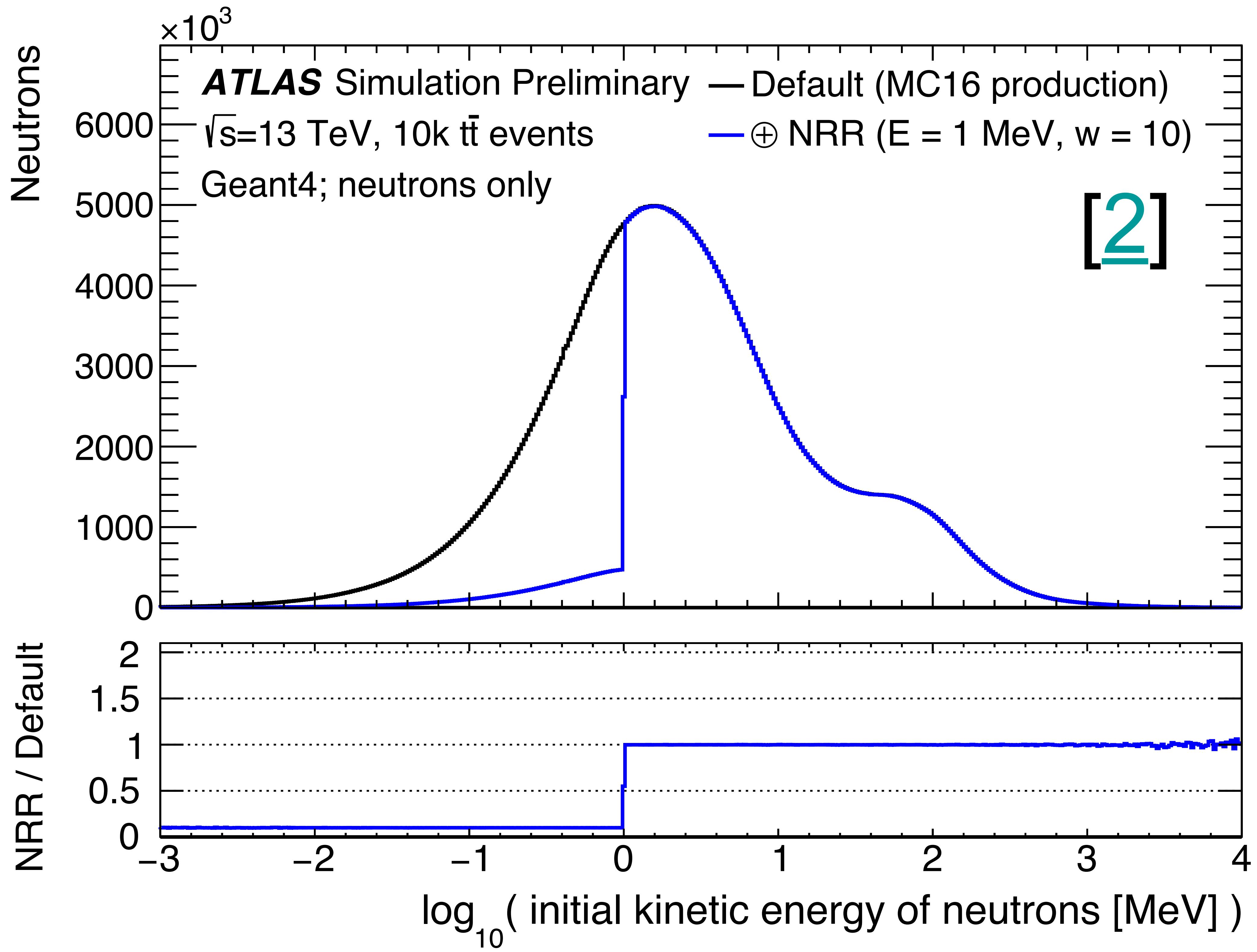
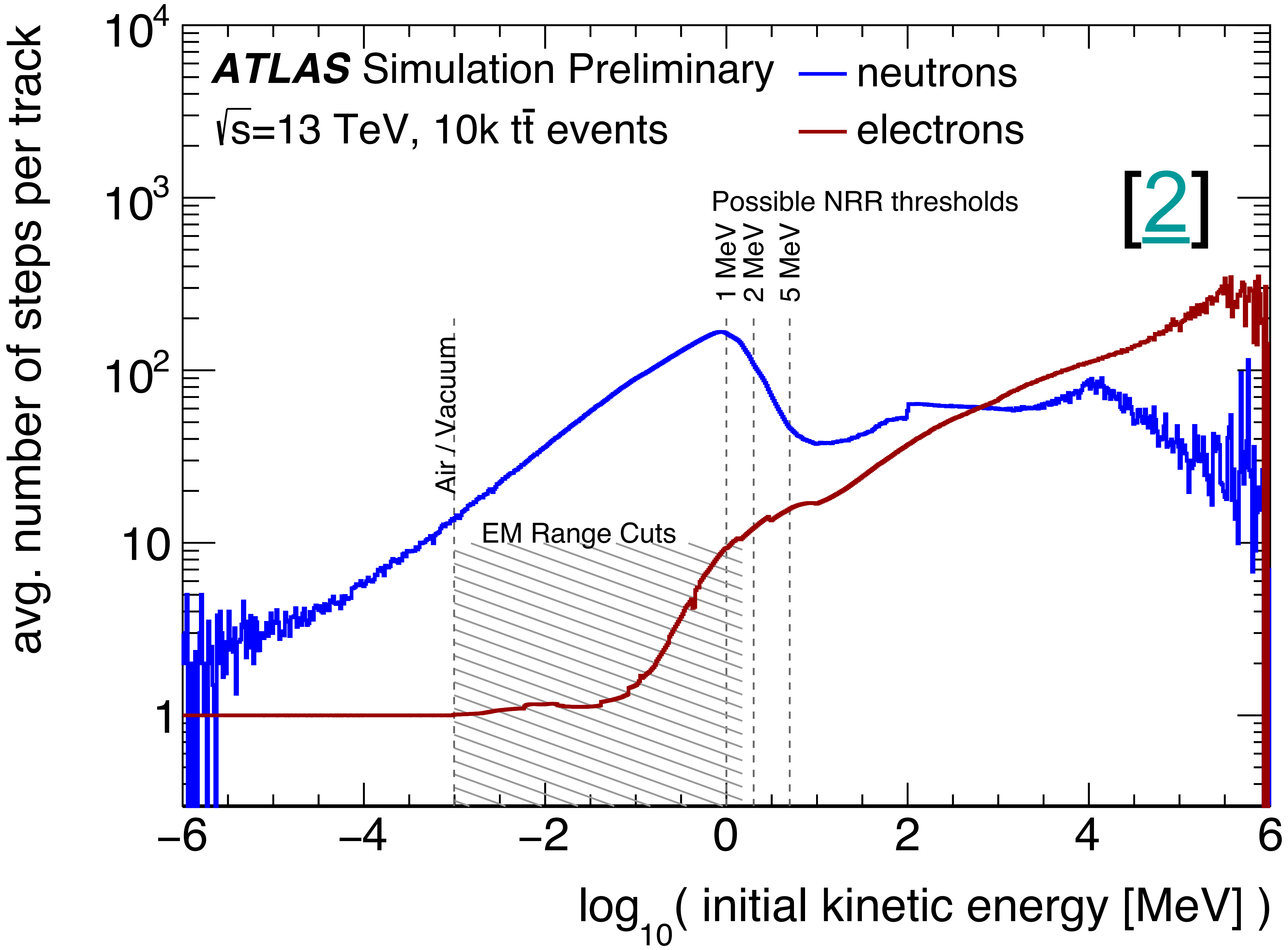


- Turning e/ɣ range cuts on decreases the amount of simulated low energy electrons by about 60%,
- A speedup of ~8% in total simulation time is achieved with this setting,
- Output is compatible with the nominal simulation.

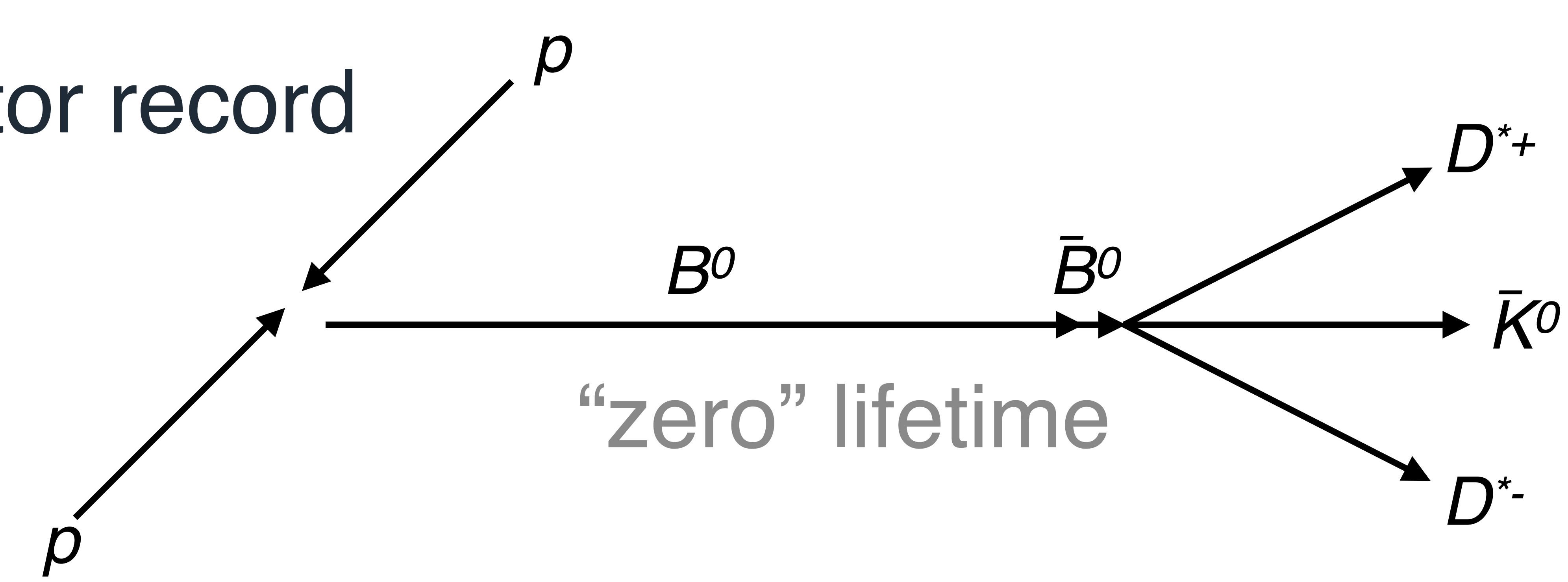
- Neutron initial kinetic energy peaks at around 1-2 MeV and neutrons with 1 MeV have the most steps on average (100-200),
- Most beneficial to 'roulette' neutrons with many steps:
  - Better CPU performance and movement less correlated to the initial point—good representation of majority,
- A NRR with a 2 MeV threshold and a weight of 10 was successfully validated a





- In generator, oscillations appear with zero lifetime,
- The oscillation vertex is added immediately before the decay vertex of the meson,
- In QS-sim, oscillation vertex is artificially positioned at the middle of the flight path during simulation and moved back on top of the decay vertex after the simulation is complete,
- Confirmed to give the desired output by flavor-tagging group in ATLAS by studying the number of pixel hits in b-jets.

Generator record



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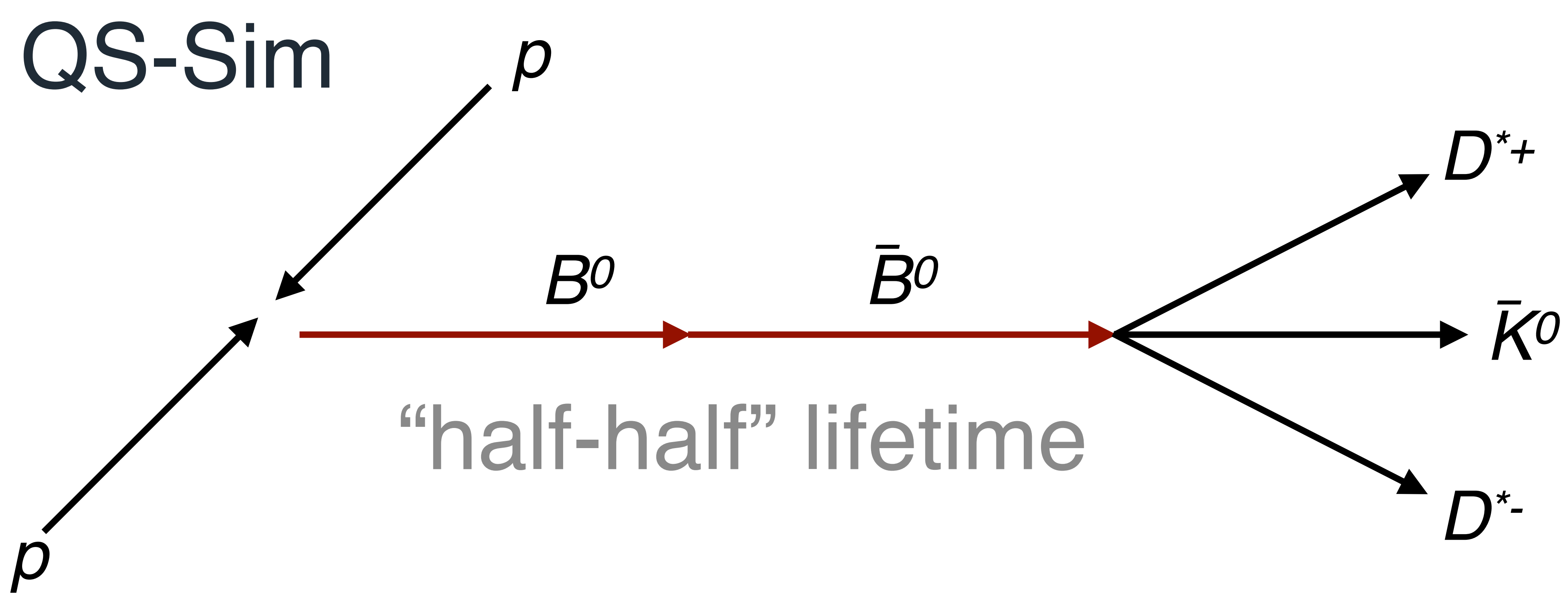
1) QS-Sim



2) Truth record