Diagnostic Plots to Study and Optimize Geometries

Miha Muškinja

HSF Detector Simulation
Thursday 12 June 2019

ATLAS EXPERIMENT

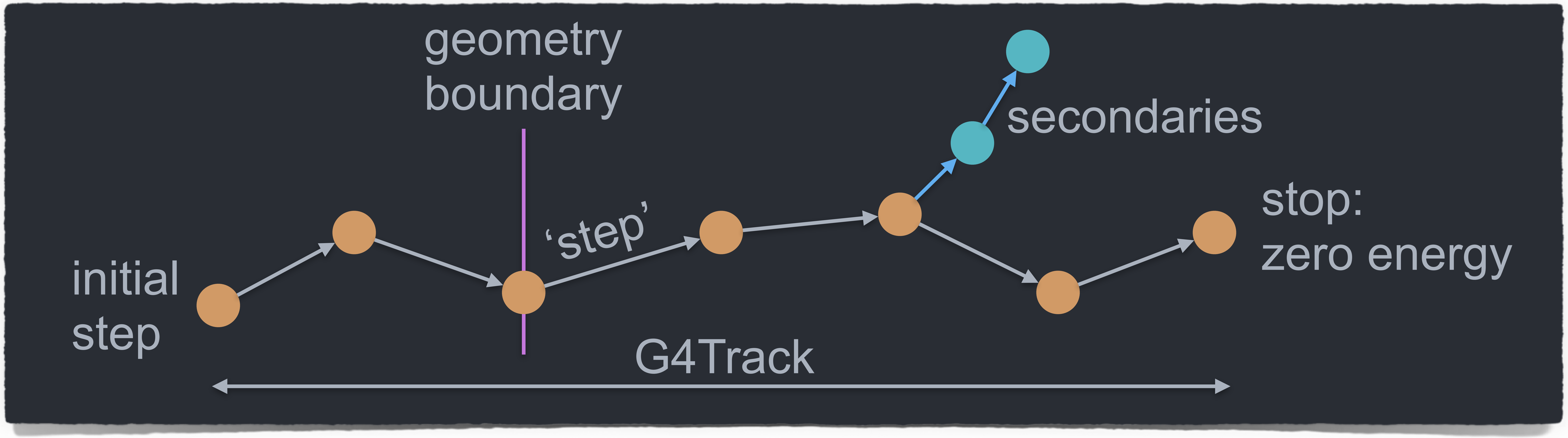
BERKELEY LAB
Lawrence Berkeley National Laboratory

Introduction

- Geant4 steps are the smallest unit of simulation and ‘stepping quantities’ (e.g. step size, energy deposit, position) are very sensitive to even the most subtle changes in Geometry (or any other changes),
  - Detailed diagnostics are very useful to immediately understand the effects and serve very well as a first pass for validation.
- Due to the very large number of Geant4 steps in ATLAS simulation (~billion per event) it is not completely trivial to create these diagnostics:
  - Impossible to save TTree-like formats; quantities have to be saved directly to histograms,
- In ATLAS, we have a specific configuration for Athena Simulation jobs that dump diagnostic / debugging plots, but make the job significantly slower,
- We study these plots for every change in the configuration, e.g.:
  - New Geant4 version, any update in geometry, performance tweaks, …

Geant4 steps

- A Geant4 process is responsible for each step, all steps of a given particle form a 'track',
- Simulation time is linearly proportional to number of steps:
  - we can speed up simulation jobs by processing fewer steps or by reducing the amount of time taken to process each step.



Example Geant4 stepping information

```
*****************************************************************************************
* G4Track Information:   Particle = e-,   Track ID = 2768138,   Parent ID = 2768092
*****************************************************************************************

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    0     42.3     24.7 -5.09e+03      16.4        0        0         0 LArMgr::LAr::Endcap::Cryostat::Cylinder::Mixed initStep
    1     41.9     23.7 -5.1e+03      12.6     3.79     9.86      9.86 LArMgr::LAr::Endcap::Cryostat::Cylinder::Mixed eIoni
    2     41.7     22.7 -5.11e+03      9.05     3.52     7.94      17.8 LArMgr::LAr::Endcap::Cryostat::Cylinder::Mixed eIoni
    3     41.7     22.7 -5.11e+03      8.53    0.053    0.157      17.9 LArMgr::LAr::Endcap::Cryostat::Cylinder::Mixed eBrem
    4     42.8     22.8 -5.11e+03      6.28     2.25     5.86      23.8 LArMgr::LAr::Endcap::Cryostat::Cylinder::Mixed eIoni
    5       45     20.3 -5.12e+03      4.63     1.65      4.7      28.5 LArMgr::LAr::Endcap::Cryostat::Cylinder::Mixed eIoni
    6     46.2     17.8 -5.12e+03      3.24      1.4     3.83      32.3 LArMgr::LAr::Endcap::Cryostat::Cylinder::Mixed eIoni
    7     45.4     15.3 -5.12e+03      2.27    0.967     3.07      35.4 LArMgr::LAr::Endcap::Cryostat::Cylinder::Mixed eIoni
    8     44.7     14.6 -5.12e+03      1.82    0.447     1.17      36.6  CALO::CALO Transportation
    9     39.9     9.24 -5.12e+03      1.82 0.000927     7.82      44.4 Atlas::Atlas Transportation
   10     34.9     2.97 -5.13e+03      1.82  0.00106     8.81      53.2    BeamPipe Transportation
   11     34.4     2.37 -5.13e+03      1.82        0    0.826        54 SectionF166 Transportation
   12     29.6    -4.65 -5.13e+03      1.62    0.199     10.5      64.5 SectionF165 Transportation
   13     29.5     -4.7 -5.13e+03      1.55   0.0718    0.235      64.7 SectionF165 msc
   14     29.3    -4.71 -5.13e+03      1.48   0.0717     0.22        65 SectionF165 msc
   15     29.1     -4.7 -5.13e+03      1.43   0.0501     0.22      65.2 SectionF165 msc
   16     28.9    -4.74 -5.13e+03      1.34   0.0891     0.22      65.4 SectionF165 msc
   17     28.8    -4.69 -5.13e+03      1.25   0.0897     0.22      65.6 SectionF165 msc
   18     28.7    -4.56 -5.13e+03      1.18   0.0649     0.22      65.8 SectionF165 msc
   19     28.6    -4.54 -5.13e+03      1.08    0.107   0.0392      65.9 SectionF163 Transportation
   20      -29    0.729 -5.12e+03      1.08 6.91e-06     61.7       128 SectionF165 Transportation
   21    -29.1    0.669 -5.12e+03      1.04   0.0398    0.135       128 SectionF165 msc
   22    -29.2    0.627 -5.12e+03      1.01    0.029    0.104       128 SectionF165 msc
   23    -29.3    0.599 -5.12e+03     0.975   0.0333    0.104       128 SectionF165 msc
   24    -29.4    0.532 -5.12e+03     0.922   0.0529    0.104       128 SectionF165 msc
   25    -29.5    0.494 -5.12e+03     0.892   0.0292    0.107       128 SectionF165 msc
```

Step properties

- Stepping quantities are extracted via a `UserSteppingAction` and saved directly in ROOT histograms,
- ‘Pre-step’ quantities are generally used. To get the corresponding physics process of a step, ‘post-step’ point has to be used.

```
// pre-step point
G4StepPoint *PreStepPoint = aStep->GetPreStepPoint();
// post-step point
G4StepPoint *PostStepPoint = aStep->GetPostStepPoint();

// pre-step volume
G4String volumeName = PreStepPoint->GetPhysicalVolume()->GetName();
// pre-step material
G4String materialName = PreStepPoint->GetMaterial()->GetName();
// process name (uses post-step point)
G4String processName = PostStepPoint->GetProcessDefinedStep();
```

https://gitlab.cern.ch/atlas/athena/blob/master/Simulation/G4Utilities/G4DebuggingTools/src/StepHistogram.cxx

Saved quantities in the UserSteppingAction

Particle name:
(e-, e+, gamma, neutron, proton, pion, other)

Volume:
(Several volumes grouped into ~20 scopes)

Material:
(First ~20 materials in number of steps)

Process:
(Save all processes)

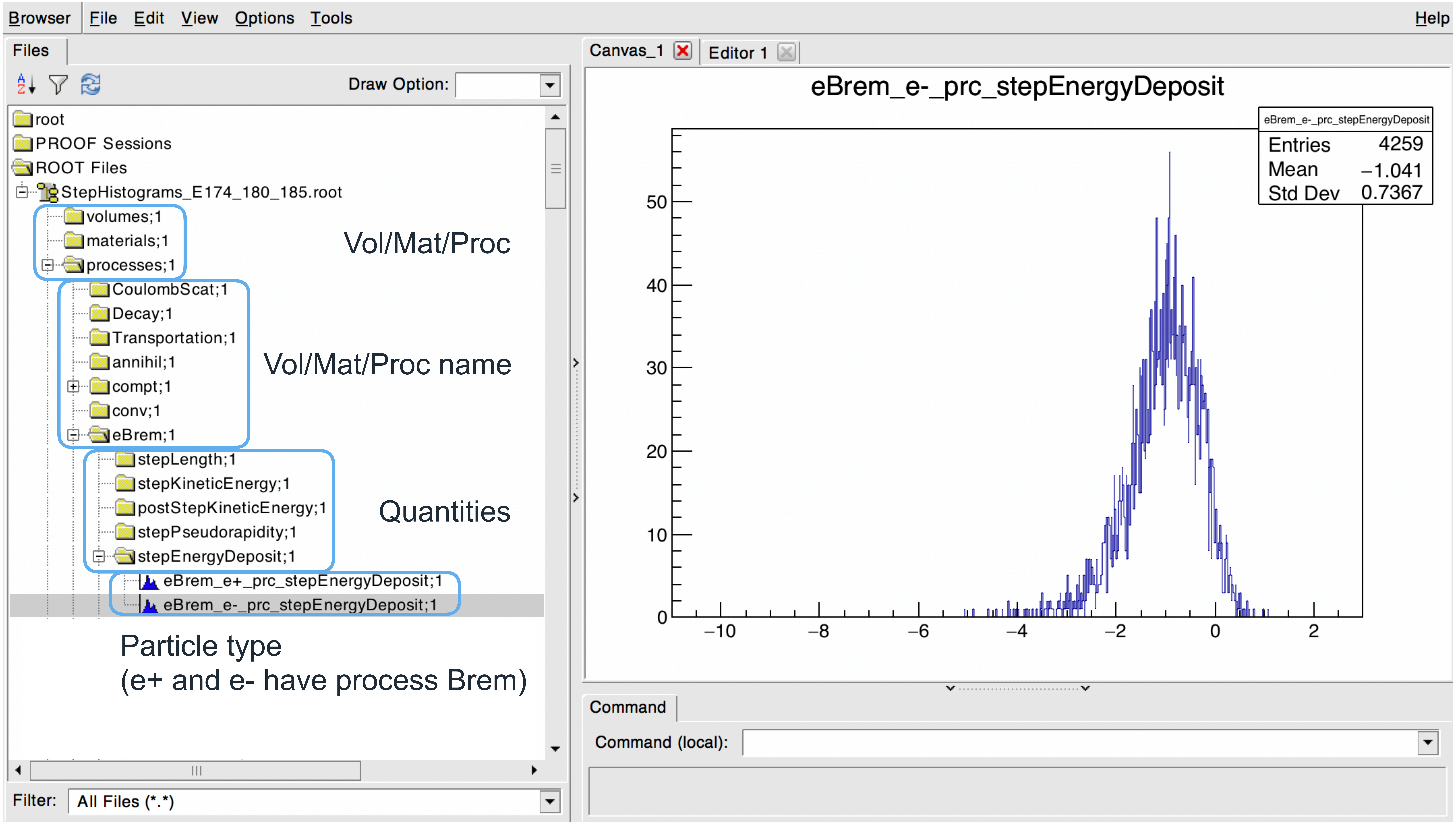
Stepping quantities:

- Pre-step kinetic energy,
- Post-step kinetic energy
- R-Z position,
- Pseudorapidity (η)
- Step length,
- Step energy deposit,
- Kinetic energy of secondaries,
- Initial kinetic energy,
- Number of steps in a track.

UserSteppingAction implementation:

https://gitlab.cern.ch/atlas/athena/blob/master/Simulation/G4Utilities/G4DebuggingTools/src/StepHistogram.cxx

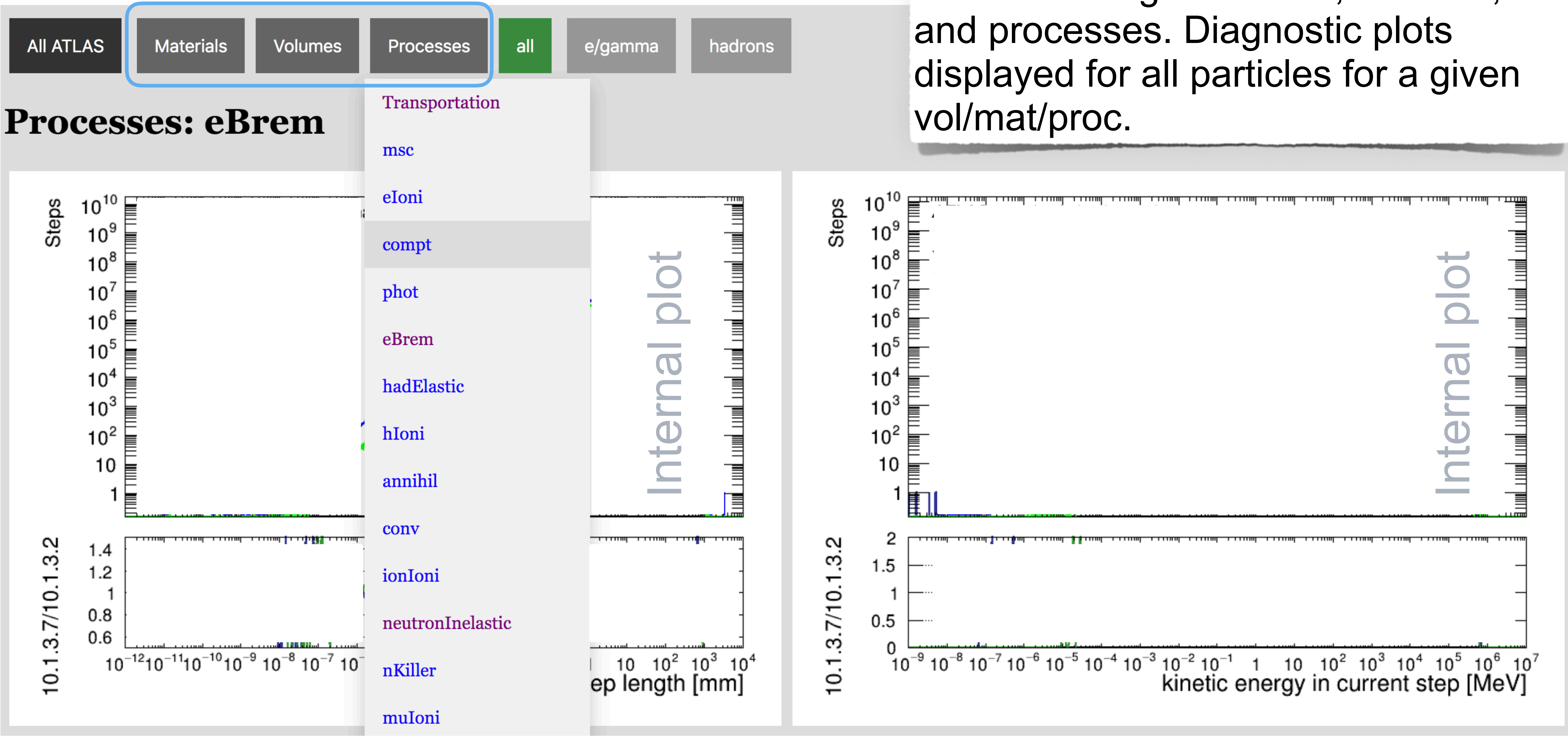
Output format— structured in folders, easily readable



Semi-automatic processing of diagnostics output

- We have a semi-automatic script to turn outputs of two simulation jobs with diagnostic plots into a browsable webpage that shows a comparison of all quantities.

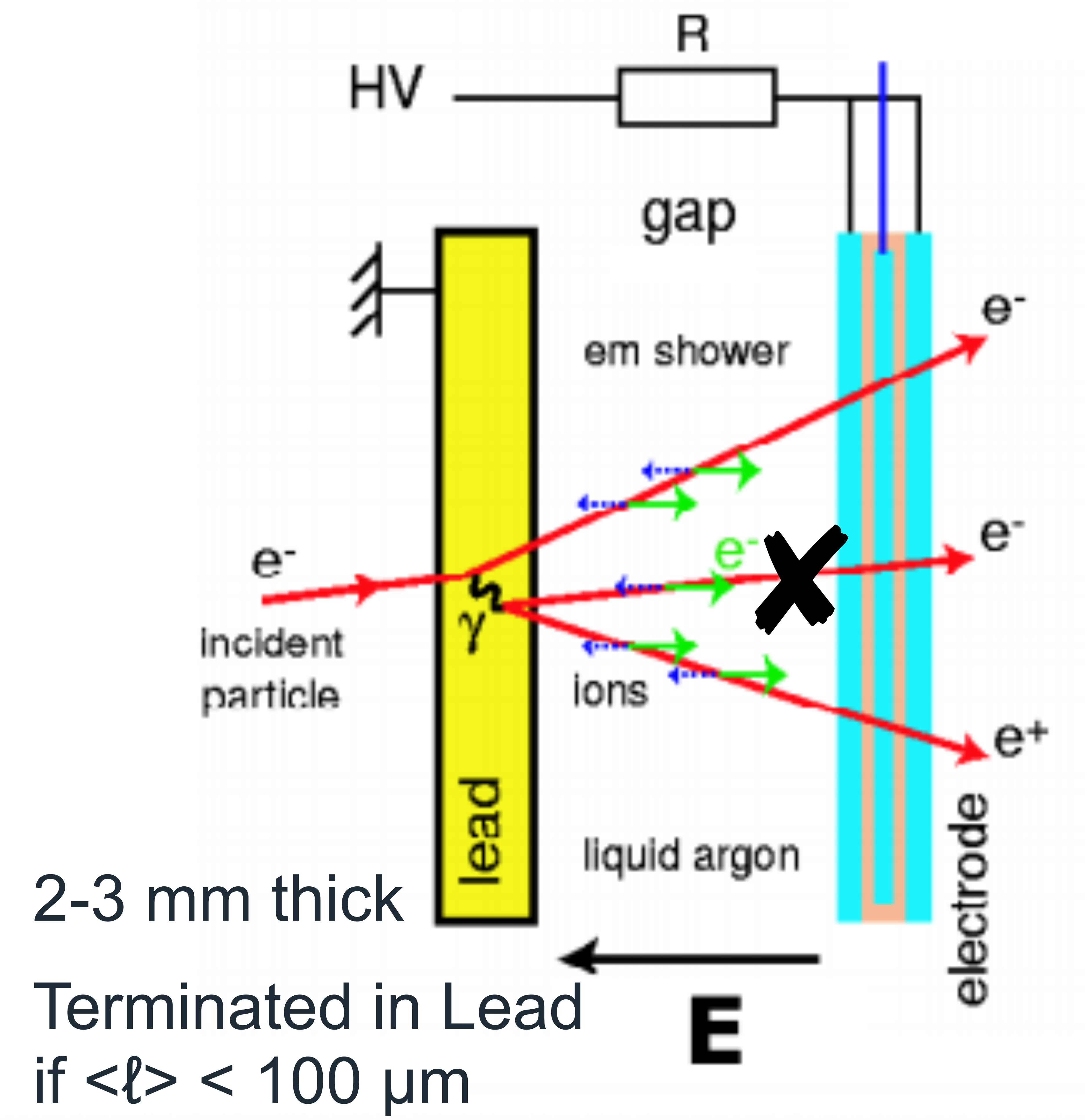
Browse through volumes, material, and processes. Diagnostic plots displayed for all particles for a given vol/mat/proc.



Examples of use-cases

- Recently we have used these plots to:
  - Optimize / evaluate a ‘Neutron Russian Roulette’ algorithm,
  - Evaluate the effect of range cuts for electromagnetic processes (‘compton’, ‘photo-electric’, and ‘conversion’),
  - Validate new versions of Geant4,
  - Check effects of geometry patches,
- The first guess and estimations are made with these diagnostic tools followed by more rigorous timing tests and full physics validation studies.

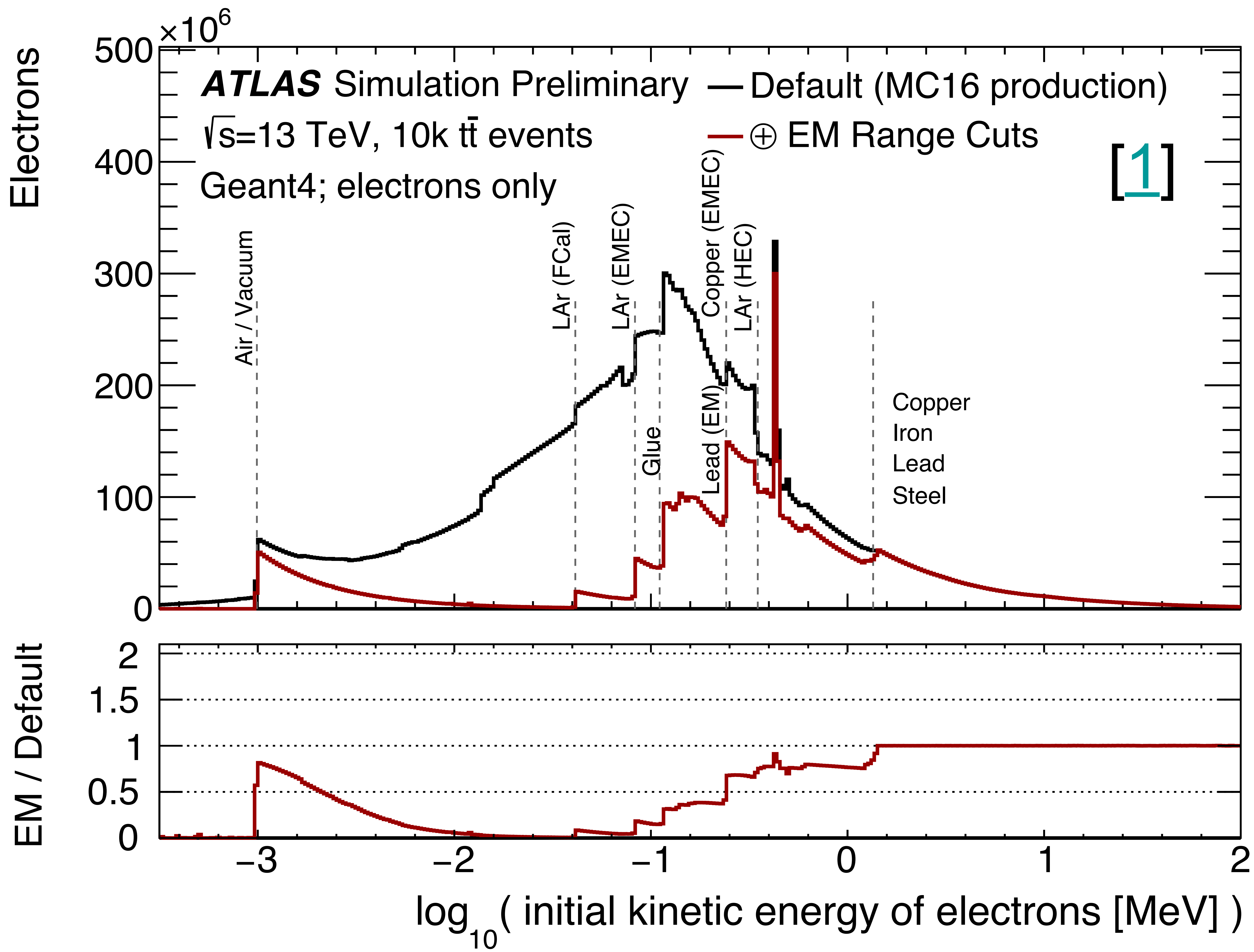
- Range cuts are a built-in way of optimizing Geant4 performance,
- For each material-volume pair, range cuts can be specified in distance units (mm),
- Secondaries, that are expected to travel less than the range cut are not created and their energy is immediately deposited by the mother particle.




```
Index : 515     used in the geometry : Yes
 Material : myLead
 Range cuts        :  gamma  100 um     e-  100 um     e+  100 um  proton 1 mm
 Energy thresholds :  gamma  29.6749 keV    e-  241.522 keV    e+  235.116 keV proton 100 keV
 Region(s) which use this couple :
    EMB
```

Range cuts for e/γ processes

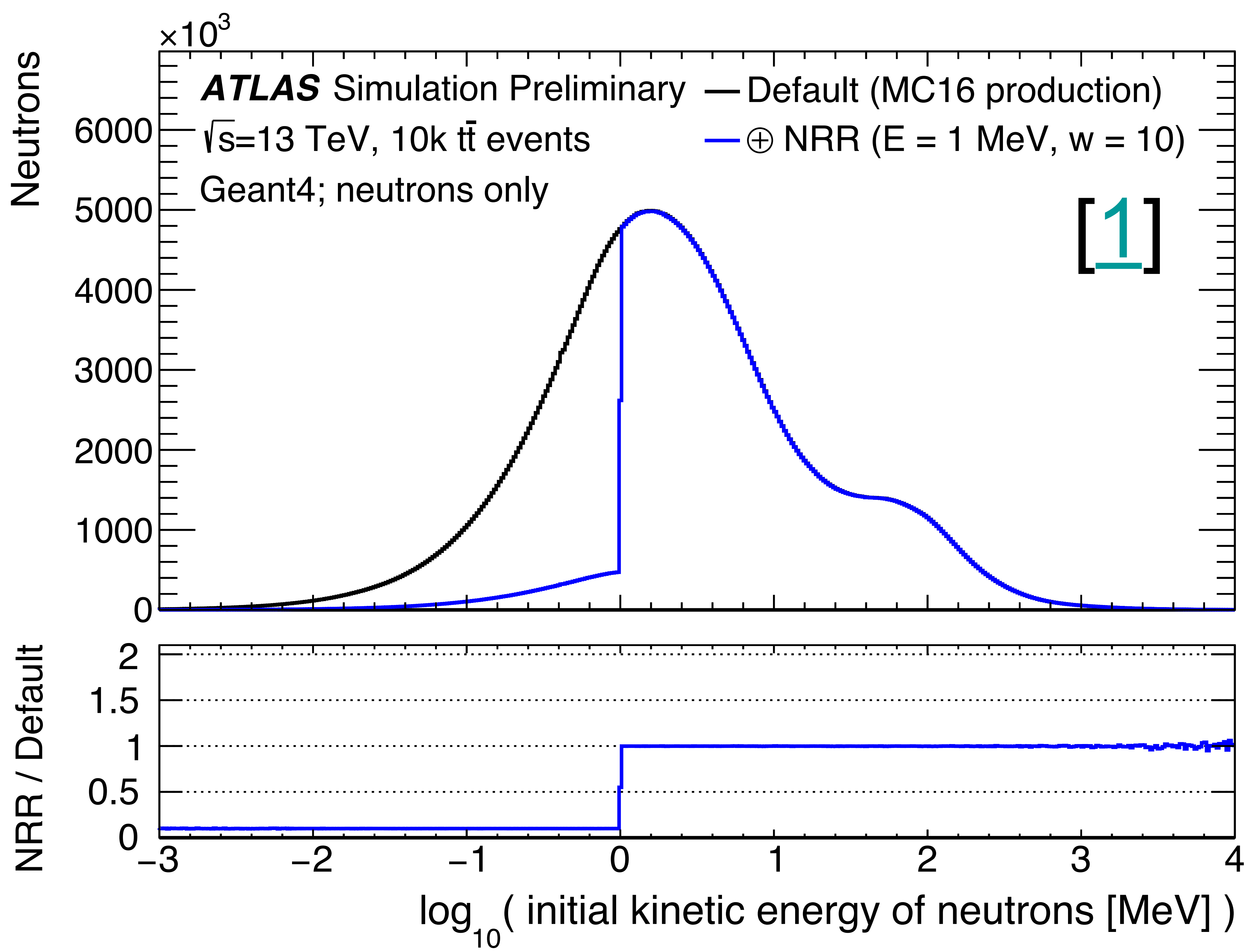
- Range cuts are off in Geant4 for 'compton', 'photo-electric', and 'conversion' processes,
- Turning them on drastically decreases the amount of simulated low energy electrons,

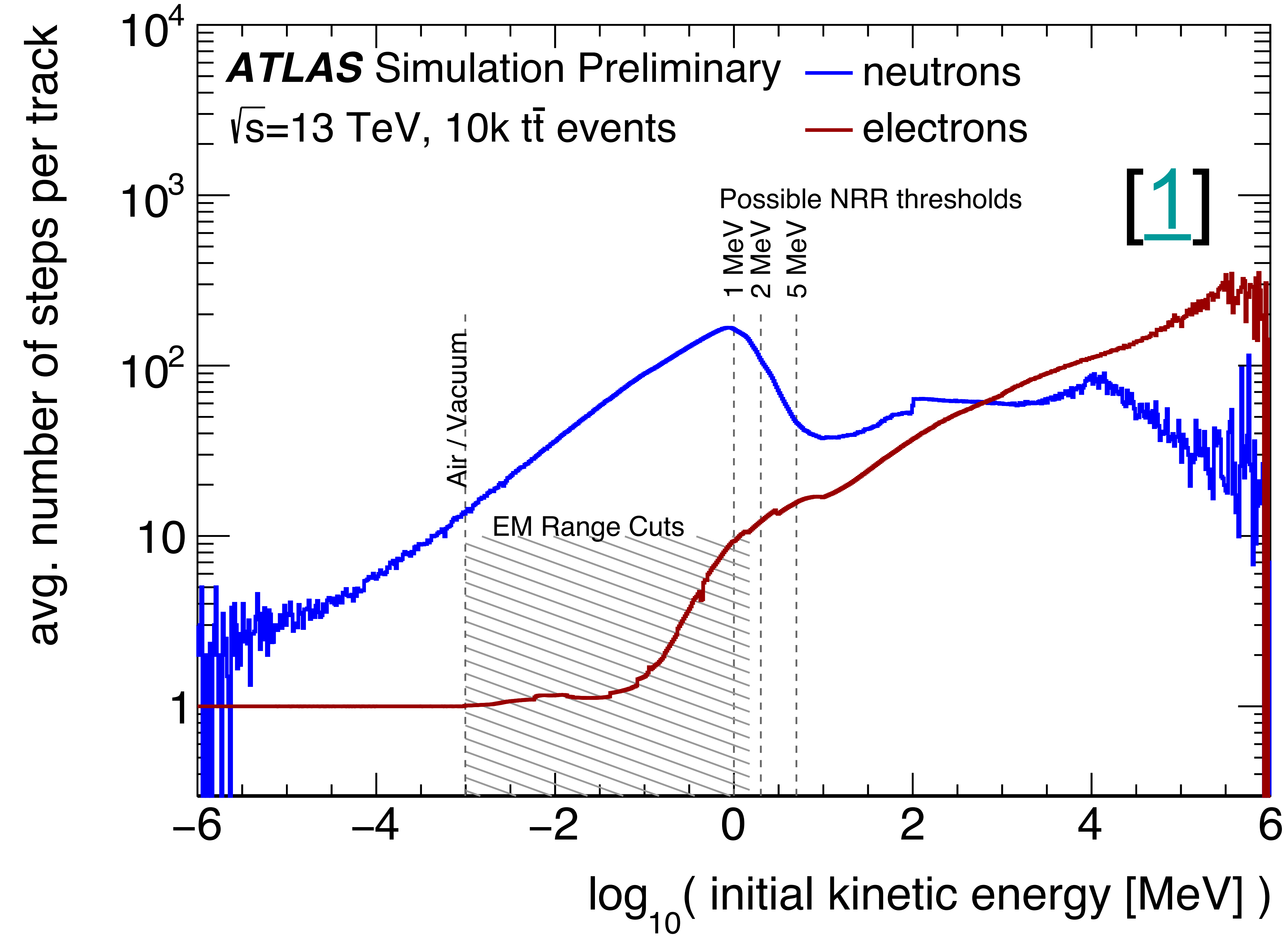


FCal = Forward Calorimeter
EMEC = Electromagnetic end-cap calorimeter
HEC = Hadronic end-cap calorimeter

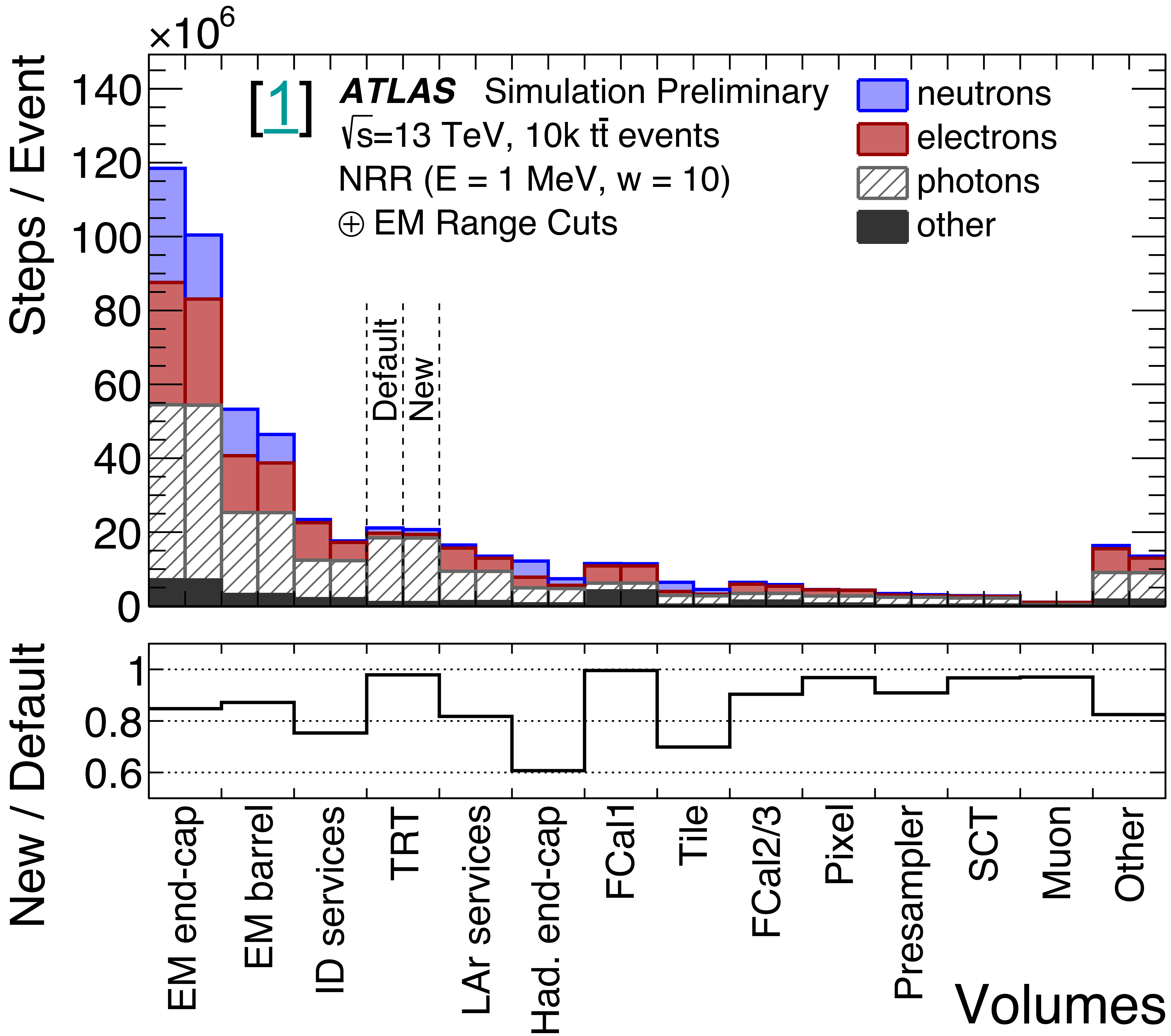
Neutron Russian Roulette performance

- Neutron initial kinetic energy peaks at around 1-2 MeV,
- Neutrons with 1 MeV have the most steps on average (100-200),
- Most beneficial to 'roulette' neutrons with many steps:
  – Better CPU performance,
  – Movement less correlated to the initial point— good representation of majority.





Most affected detector volumes



- Pre-calculated shower libraries in FCal for electrons, photons, and neutrons (frozen showers) are included in these jobs,
- Most of simulation time is spent in LAr calorimeters, ID services + beampipe, and TRT,
- Photons produce the most steps, followed by electrons and neutrons,
- With a [1 MeV, w = 10] NRR and EM range cuts, we get 20-40% fewer steps in calorimeters,

EM = Electromagnetic (calorimeter), ID = Inner Detector, FCal = Forward Calorimeter, TRT = Transition Radiation Tracker

Summary

- ATLAS has Athena algorithms that dump O(1000) diagnostic plots in a simulation job related to stepping quantities,
  - Diagnostic plots are made for each particle and grouped into Volumes, Materials, and Processes.
  - Semi-automatic scripts are used to transform the ROOT output into human-digestible plots / webpage.
- These diagnostic tools are very useful to immediately see the effect of any new geometry patch, Geant4 version, etc..
  - Stepping quantities are very sensitive to even the smallest changes in configuration and usually give a good understanding of the effects.

BACKUP

Neutron Russian Roulette

- Randomly discard neutrons below some energy and weight the energy deposits of remaining neutrons accordingly:
  - Energy Threshold (E_{th}),
  - Weight (w): neutrons below E_{th} are discarded with P((w-1)/w) and energy deposits of remaining neutrons are multiplied by w.
- We believe we can do this because neutrons make lots of steps so we think we can approximate the response with a subset.