Fast simulation in Geant4

A. Zaborowska, EP-SFT

GEANT4 R&D meeting

25/06/2019

Outline

Why fast(er) simulation?

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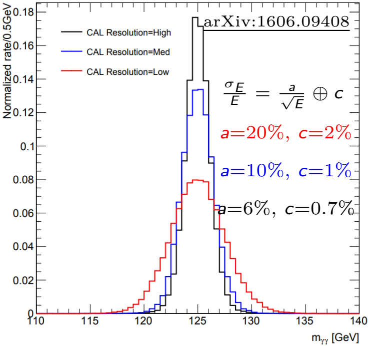
physics studies that assume certain detector performance



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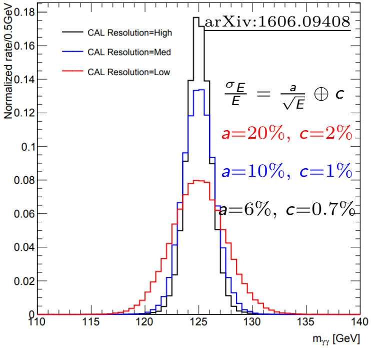
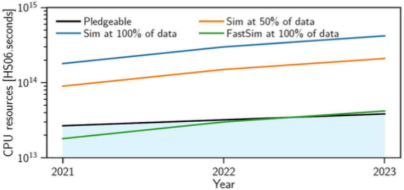
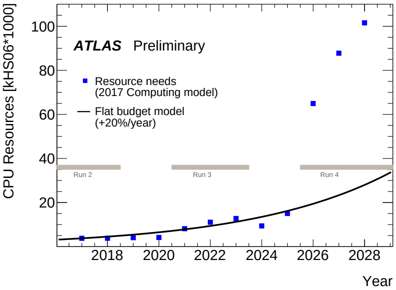
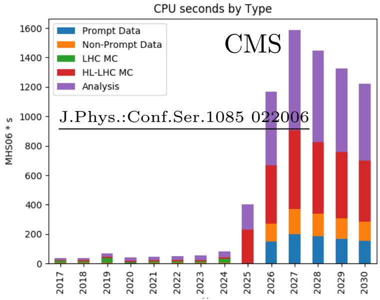


G. Corti, HSF2018, Naples



ATLAS Public





more data (⇒ CPU time) needed

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- Some of existing 'users' of fast simulation in Geant4:
  - FCC - parametric (smearing of properties, GFlash) - allows flexibility with mixing full and fast sim
  - LHCb - first tests with `G4VFastSimulationModel`

    shower libraries (CERN-THESIS-2018-293)

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    shower libraries (CERN-THESIS-2018-293)
- Different approaches used: parametrisation, shower libraries
- Being explored: machine learning techniques

Status in Geant4

- Fast simulation utilities
  - `G4FastSimulationManagerProcess`
  - since v10.3 `G4FastSimulationPhysics`
  - `G4Region` - *where*
  - `G4VFastSimulationModel` - *what*

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  - `G4Region` - *where*
  - `G4VFastSimulationModel` - *what*
  - messenger:

```
/param/ // Fast Simulation print/control commands.
/param/showSetup // Show fast simulation setup (for each world: fast simulation
↪ manager process - which particles, region hierarchy - which models)
/param/listEnvelopes <ParticleName (default:all)> // List all the envelope names
↪ for a given particle (or for all particles if without parameters).
/param/listModels <EnvelopeName (default:all)> // List all the Model names for a
↪ given envelope (or for all envelopes if without parameters).
/param/listIsApplicable <ModelName (default:all)> // List all the Particle names
↪ a given model is applicable (or for all models if without parameters).
/param/ActivateModel <ModelName> // Activate a given Model.
/param/InActivateModel <ModelName> // InActivate a given Model.
```

Models

- GFlashShowerModel - the only existing implementation in 'core' Geant4
- Several example models in examples/extended/parameterisations/:
  - Par01
    - Par01EMShowerModel
    - Par01PionShowerModel
    - Par01PiModel
  - Par02
    - Par02FastSimModelEMCal
    - Par02FastSimModelHCal
    - Par02FastSimModelTracker

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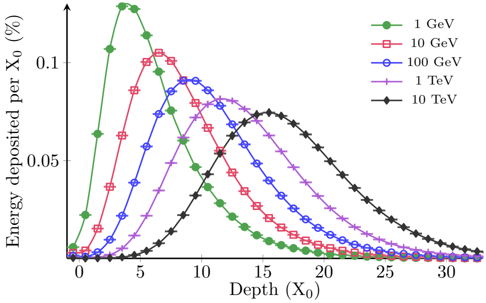
- t and r are expressed in units of X_0 and R_M

Example 3 - longitudinal profile



$$T \sim \ln E$$

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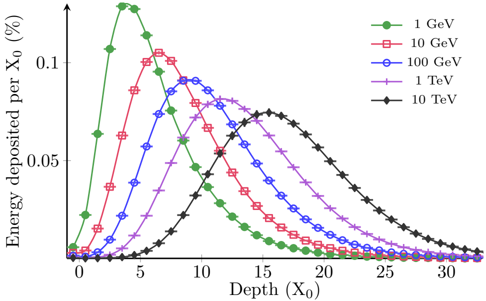

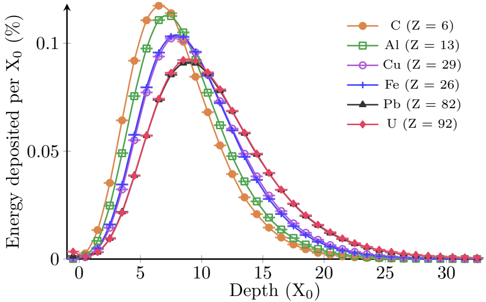

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A.1 Homogeneous Media

A.1.1 Average longitudinal profiles

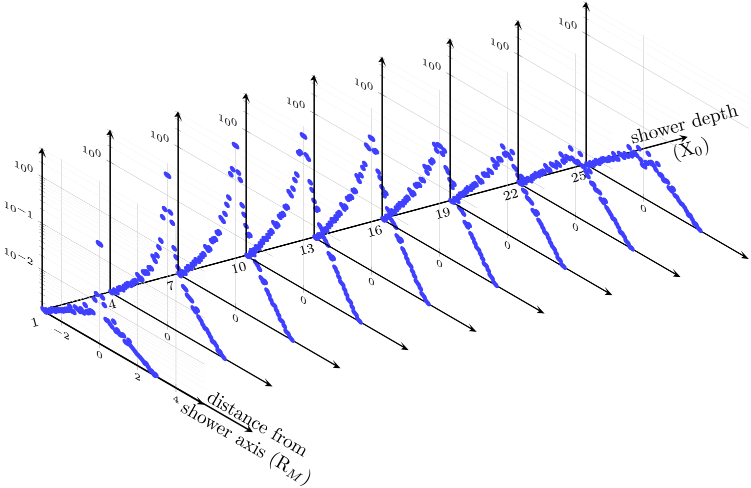
$$\begin{aligned} T_{hom} &= \ln y - 0.858 \\ \alpha_{hom} &= 0.21 + (0.492 + 2.38/Z) \ln y \end{aligned}$$

A.1.2 Fluctuated longitudinal profiles

$$\begin{aligned} \langle \ln T_{hom} \rangle &= \ln(\ln y - 0.812) \\ \sigma(\ln T_{hom}) &= (-1.4 + 1.26 \ln y)^{-1} \\ \langle \ln \alpha_{hom} \rangle &= \ln(0.81 + (0.458 + 2.26/Z) \ln y) \\ \sigma(\ln \alpha_{hom}) &= (-0.58 + 0.86 \ln y)^{-1} \\ \rho(\ln T_{hom}, \ln \alpha_{hom}) &= 0.705 - 0.023 \ln y \end{aligned}$$

arXiv:hep-ex/0001020

Example 3 – lateral profile



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Description dependent on $\tau = \frac{t}{T}$:

$$R_{\mathrm{core}}(\tau) = r_1 + r_2\tau$$

$$R_{\mathrm{tail}}(\tau) = r_3 \left(\mathrm{e}^{r_4(\tau - r_5)} + \mathrm{e}^{r_6(\tau - r_7)}\right)$$

$$p(\tau) = r_8 \exp\left(\frac{r_9 - \tau}{r_{10}} - \exp\left(\frac{r_9 - \tau}{r_{10}}\right)\right)$$

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A.1.3 Average radial profiles

$$R_{C,hom}(\tau) = z_1 + z_2\tau$$
$$R_{T,hom}(\tau) = k_1\{\exp(k_3(\tau - k_2)) + \exp(k_4(\tau - k_2))\}$$
$$p_{hom}(\tau) = p_1 \exp\left\{ \frac{p_2 - \tau}{p_3} - \exp\left(\frac{p_2 - \tau}{p_3} \right) \right\}$$

with

$$z_1 = 0.0251 + 0.00319 \ln E$$
$$z_2 = 0.1162 + -0.000381 Z$$
$$k_1 = 0.659 + -0.00309 Z$$
$$k_2 = 0.645$$
$$k_3 = -2.59$$
$$k_4 = 0.3585 + 0.0421 \ln E$$
$$p_1 = 2.632 + -0.00094 Z$$
$$p_2 = 0.401 + 0.00187 Z$$
$$p_3 = 1.313 + -0.0686 \ln E$$

A.1.4 Fluctuated radial profiles

$$\tau_i = \frac{t}{\langle t \rangle_i} \frac{\exp(\langle \ln \alpha \rangle)}{\exp(\langle \ln \alpha \rangle) - 1}$$
$$N_{Spot} = 93 \ln(Z) E^{0.876}$$
$$T_{Spot} = T_{hom}(0.698 + 0.00212 Z)$$
$$\alpha_{Spot} = \alpha_{hom}(0.639 + 0.00334 Z)$$

arXiv:hep-ex/0001020

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- sampling calorimeter treated as effective medium
- material distribution in the sampling calorimeter taken into account (in paper, is it already implemented in G4?)

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   - locate volume, check if SD, add to hit collection

Homogeneous calorimeter

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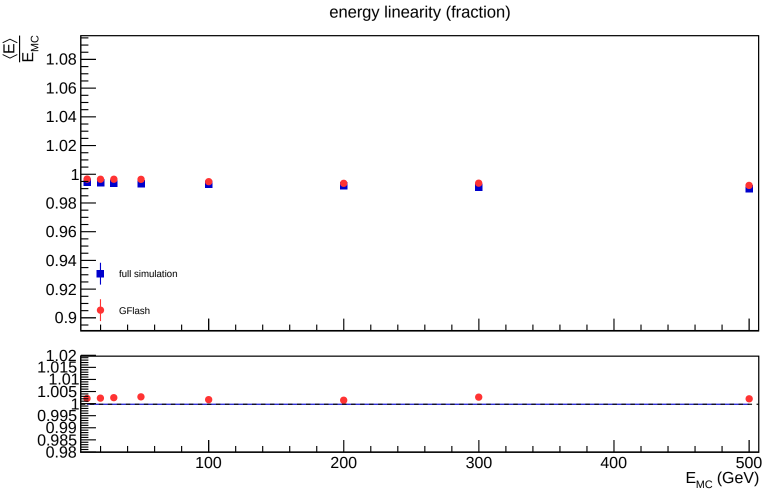
- comparison of GFlash to the full simulation:
  - total deposited energy and longitudinal profile well reproduced (few %)
  - accuracy of the transverse profile ~20%
  - energy deposited in $2-3$ times less cells
  - simulation speed-up independent on energy

    (time spent mostly in volume look-up: higher E = more cells)

Homogeneous calorimeter



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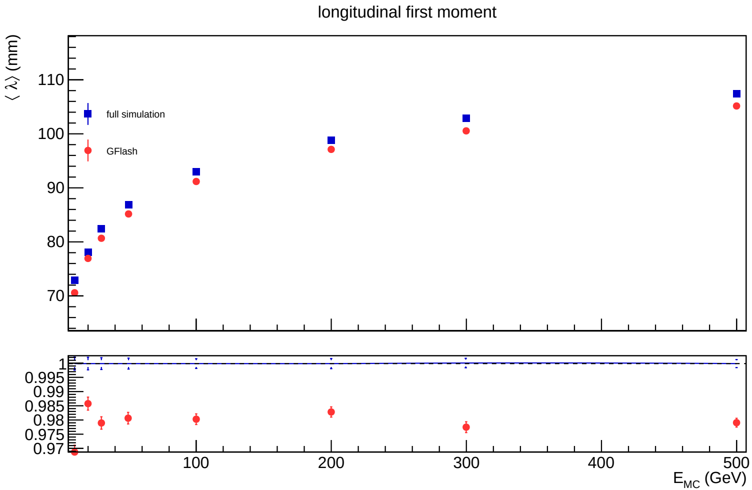

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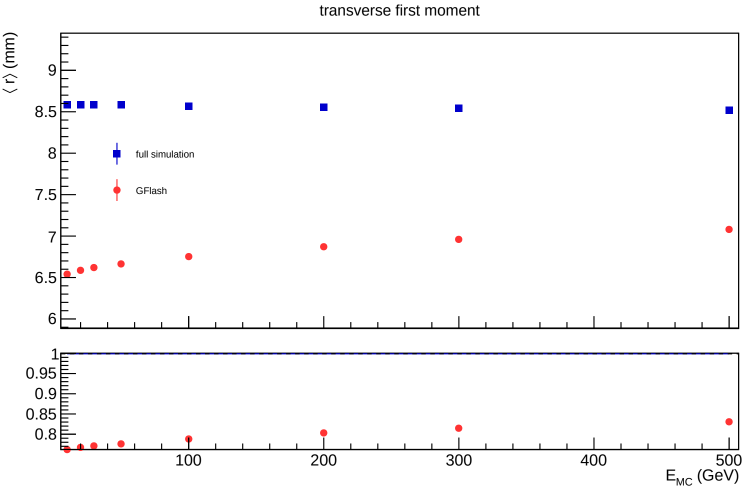

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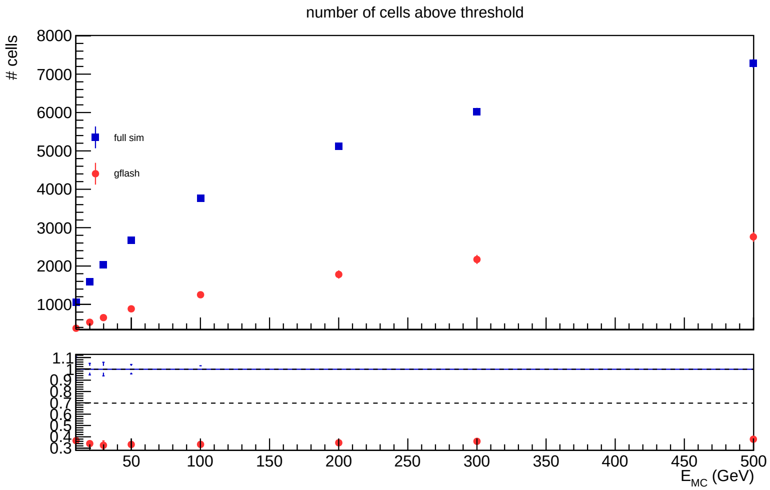

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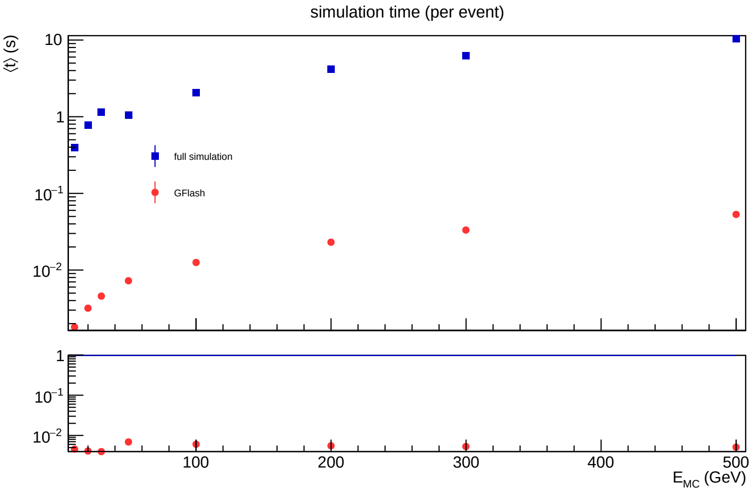

Sampling calorimeter

- SiW sampling calorimeter (1.9 mm W, 0.5 mm Si)
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- comparison of GFlash to the full simulation:
  - no distinction of the material distribution

    $4-6$ times more energy deposited in Si than in full simulation

    not visible if deposit from both active and passive material is registered

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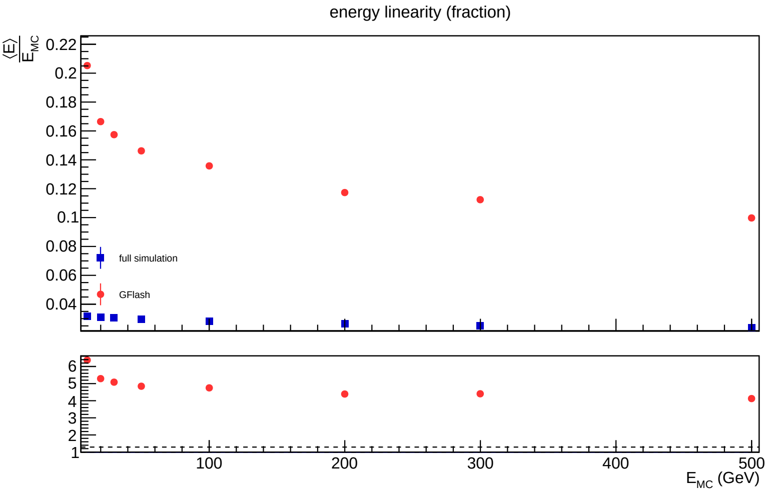

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- Introduce e.g. parametrisation of shower start point
- In contact with CMS (GFlash-like parametrisation), gain from their experience

Machine learning techniques

- Basic idea: do not use given formulas to describe showers, instead learn the relations and reproduce them
- Developed in many experiments/detectors (network architecture, training)
  - Principle Component Analysis (PCA)
  - Generative Adversarial Networks (GAN)
  - Variational Auto-Encoders (VAE)
  - ... (Ioana's talk)

    HSF-simulation 6/03/2019

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- Integration with main framework (C++) necessary (inference)
- Use Geant4 to generate samples, validate trained network, use inferred showers within simulation

What is needed?

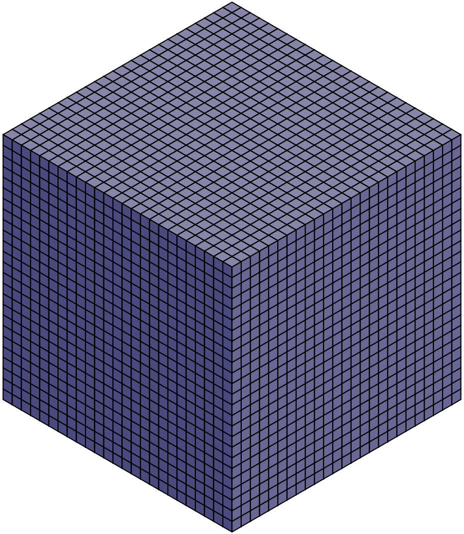
1. Data of calorimeter showers (from GEANT4) in a studied detector
2. Neural network
3. Training of 2) using 1)
4. Extraction of trained weights
5. Application in the simulation

   instead of calculating profiles - infer shower using imported DNN architecture and weights

Generation of data and validation

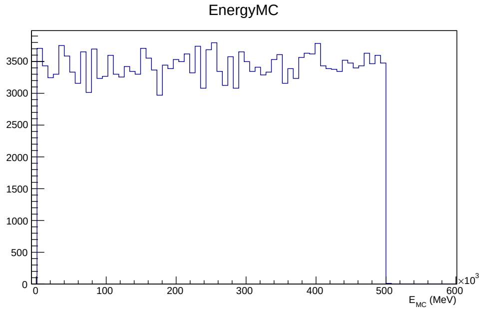
- Simple example for data generation in configurable detector setups
- Based on many existing examples/tests
- Can be integrated as one of the examples
- Validation plots presented for GFlash

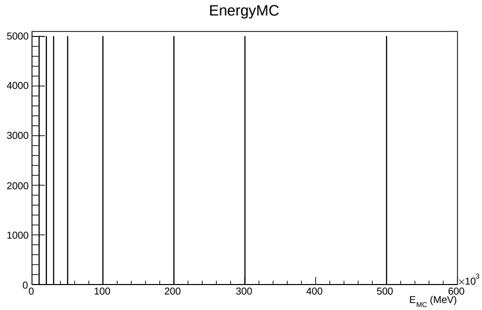
Detector



- net of $N \times N \times M$ cells
  - N in xy plane, M along z axis
  - $25 \times 25 \times 25$ for current ML studies
- each cell can be build of K absorbers (TestEm3 inspired) perpendicular to particle direction
  - $K = 1$ for homogeneous calorimeters, e.g.. $PbWO_4$
  - other geometries: Pb/LAr, Pb/Sci, W/Si (SimplifiedCalorimeter inspired)
- using detector messenger to set size, number of cell, materials, sensitivity
- current cell size: $\sim 1X_0$ in z and $\sim 0.5R_M$ in xy

Particle generator





- flat energy spectrum (1–500 GeV) of particle gun along z axis
- for ML training

- single energy particle gun along z axis
- for validation/ analysis/ comparison

Next step: varied angle (both for training and validation)

Simulation type

- full simulation (FTFP_BERT, easy to change if needed)

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  - using existing implementation (parameters)
  - implemented in G4 for e^-, e^+

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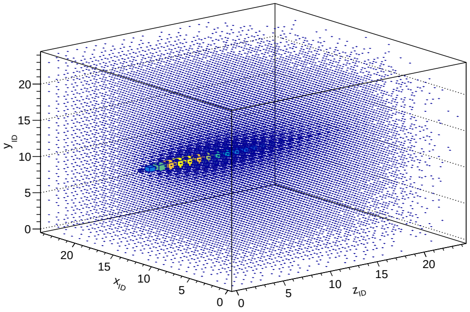
- GFlash parametrisation:
  - using existing implementation (parameters)
  - implemented in G4 for e^-, e^+
- NN inference (not yet available...)

Output

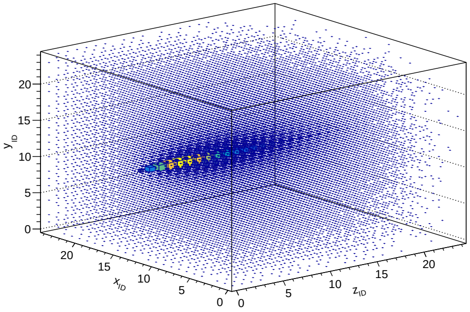
- creating ntuples using G4AnalysisManager
- stored in ROOT files



Output

- creating ntuples using G4AnalysisManager
- stored in ROOT files
- investigation of storing to H5

  directly from GEANT4



- currently for ML studies: created simple tools for ROOT↔H5 translation of cell energy map
  - HDF5 stores datasets – multidimensional arrays of a homogeneous type
  - quick to read in python for ML training (as numpy arrays)

Validation

Set of general validation histograms is created:

- MC energy
- deposited energy
- number of cells above threshold (currently $E_{\text{cell}} > 0.1$ MeV)
- cell energy distribution
- longitudinal and transverse profiles (and first/second moments)
- energy distribution layer-wise
- transverse profile layer-wise
- simulation time

Gaussian distributions (deposited energy, shower moments) can be additionally fitted and plotted as a function of MC energy.

Neural Network

see Ioana's presentation

Inference

- Training with Python
- Store model and trained weights

Inference

- Training with Python
- Store model and trained weights
- Integration in C++ frameworks necessary for use in event simulation
- Inference
  - not detector specific
  - could be a (second) `G4VFastSimulationModel` implementation,

    e.g. available in Geant4 if compiled against NN-aware toolkit

    (like HDF5 in the analysis)

Summary

On-going work...

- shower parametrisation development
  - investigate and address the sampling calorimeter issues
  - efficient creation of deposits/location of volumes
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  - validation tools
  - inference within Geant4
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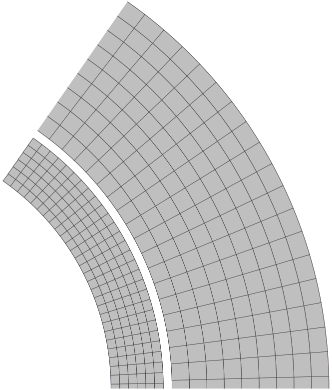
Other areas of fast simulation:

- fast track simulation
- full simulation optimisation (e.g. applying biasing techniques)

Additional slides

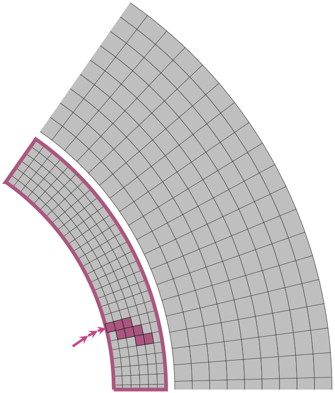
Example Par01

Time consuming simulation of calorimeters replaced by creation of energy deposits.



Example Par01

Time consuming simulation of calorimeters replaced by creation of energy deposits.

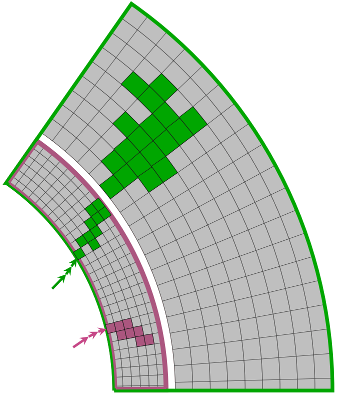


Par01EMShowerModel.cc

- electrons and photons
- electromagnetic calorimeter, envelope in mass geometry

Example Par01

Time consuming simulation of calorimeters replaced by creation of energy deposits.



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Par01PionShowerModel.cc

- pions
- both calorimeters: envelope around EMCal and HCal
  $\Rightarrow$ parallel geometry

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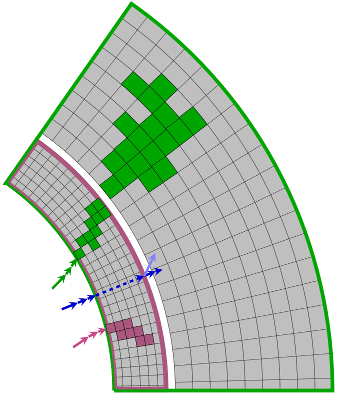

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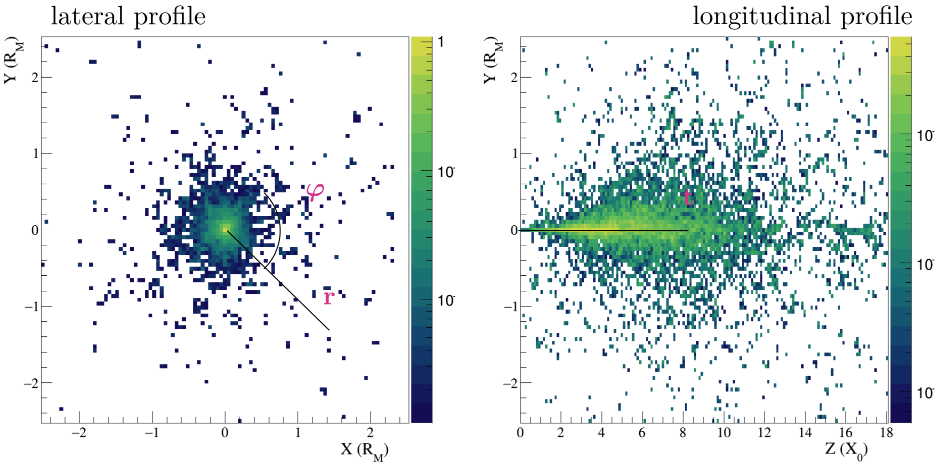
`Par01PionShowerModel.cc`

- pions
- both calorimeters: envelope around EMCal and HCal
  ⇒ parallel geometry

`Par01PiModel.cc`

- create secondaries

Shower profiles



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How to deposit energy E of electrons/photons?

Par01EMShowerModel.cc

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$$f(t, r, \varphi) = f(t)f(r)f(\varphi)$$

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   in $(t$,r,$\varphi)$ inside electromagnetic calorimeter

Par01PionShowerModel

How to deposit energy E of pions?

Par01PionShowerModel.cc

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$$f(x,\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2 / 2\sigma^2}$$

1. longitudinal shower profile $f(t, 0, 20\text{cm})$
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   in (t,r,φ) inside electromagnetic + hadronic calorimeter envelope

Example Par02

- Simple parametrisation

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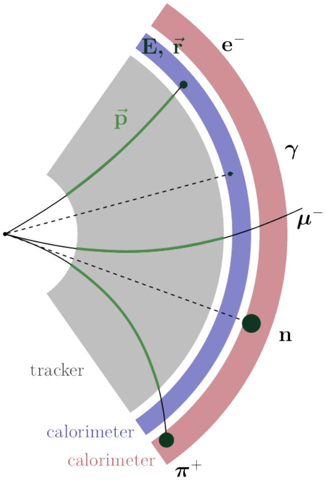

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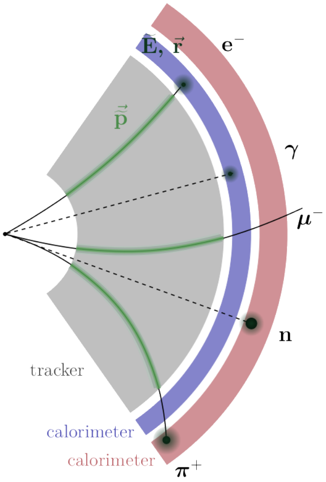

- Simple parametrisation
- Smearing of the momentum in the tracker and energy in the calorimeter

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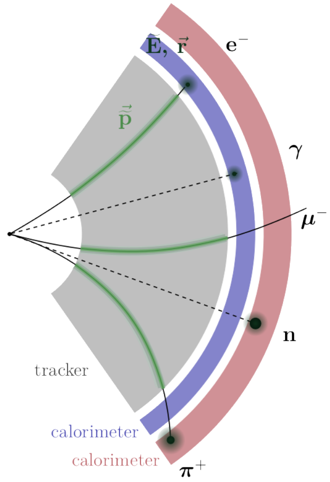

- Simple parametrisation
- Smearing of the momentum in the tracker and energy in the calorimeter
- User input: detector resolution;

$$\sigma_{p_T} = 1.3\%$$

$$\sigma_E = \frac{110\%}{\sqrt{E}} \oplus 9\%$$

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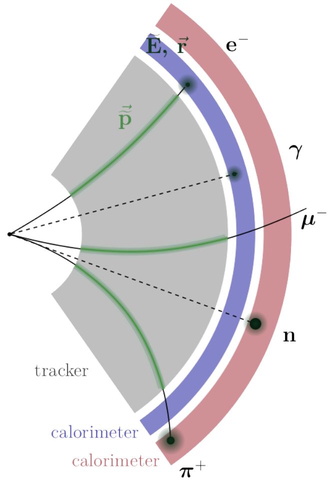

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