Ideas for accelerating EM physics simulation in HEP

Electromagnetic Plenary Session at 27th GEANT4 Collaboration Meeting

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Contents

Woodcock tracking in GEANT4

Combining transportation and Multiple Scattering

Update on G4HepEm

Conclusions

Woodcock tracking in GEANT4

- Interactions added as separate processes
  - Rayleigh, photoelectric, Compton, conversion, gamma-nuclear, ...
  - Corresponding *macroscopic cross sections* $\Sigma_\gamma^p(E, \text{material})$

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  - Path length till the next interaction follows exponential distribution: $s_p(E, \text{material}) \sim \mathbb{E}\text{xp}\left[\Sigma_\gamma^p(E, \text{material})\right]$
- Select shortest proposed step length: $s(E, \text{mat}) = \min\left\{s_p(E, \text{mat})\right\}$
  - BUT: track must be stopped at volume boundary / material change
  - To reevaluate cross sections, compute new path length, ...

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- Advantage: only evaluate *total macroscopic cross section* at pre-step point $\Sigma_\gamma(E, \mathrm{material}) = \sum_p \Sigma_\gamma^p(E, \mathrm{material})$
- Only need to evaluate individual cross sections if interaction happens during step $P_p(E, \mathrm{material}) = \Sigma_\gamma^p(E, \mathrm{material}) / \Sigma_\gamma(E, \mathrm{material})$

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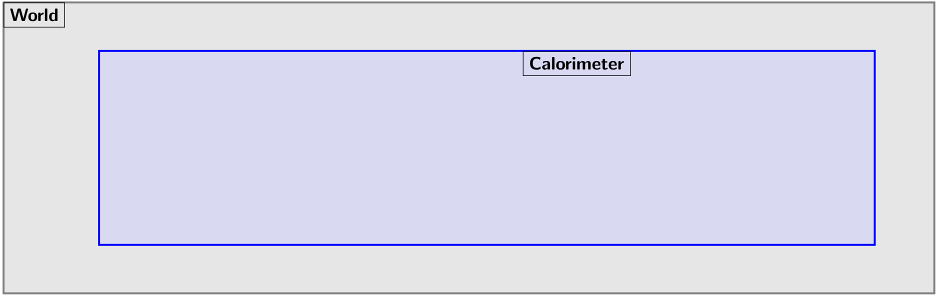
- Introduce "artificial" δ-interaction with $\Sigma_\delta(E, \mathrm{mat}) = \mathit{const.} - \Sigma_\gamma(E, \mathrm{mat})$
- Thus $\Sigma(E) = \Sigma_\gamma(E, \mathrm{mat}) + \Sigma_\delta(E, \mathrm{mat}) = \mathit{const.}$ across materials
  - Step length $s(E) \sim \mathbb{E}\mathrm{xp}\left[\Sigma(E)\right]$ till next real or δ-interaction
  - Real interaction happens with probability $P_\gamma(E, \mathrm{mat}) = \Sigma_\gamma(E, \mathrm{mat})/\Sigma(E)$

Woodcock tracking in GEANT4

Example



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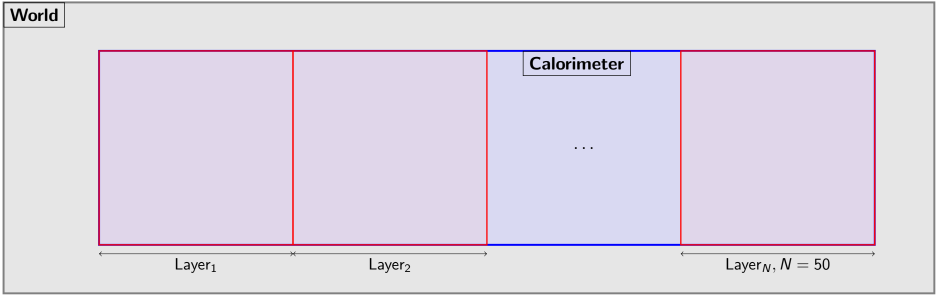

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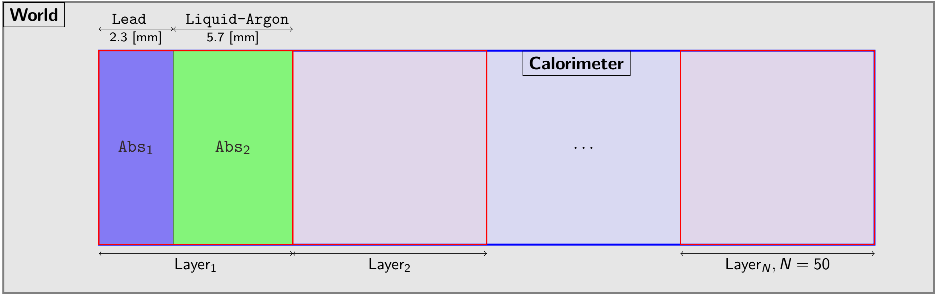

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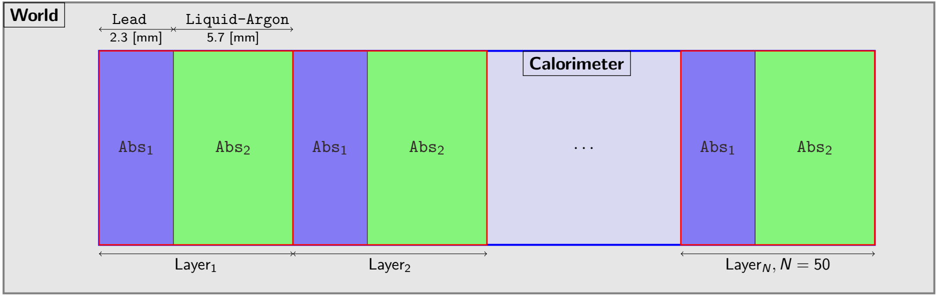

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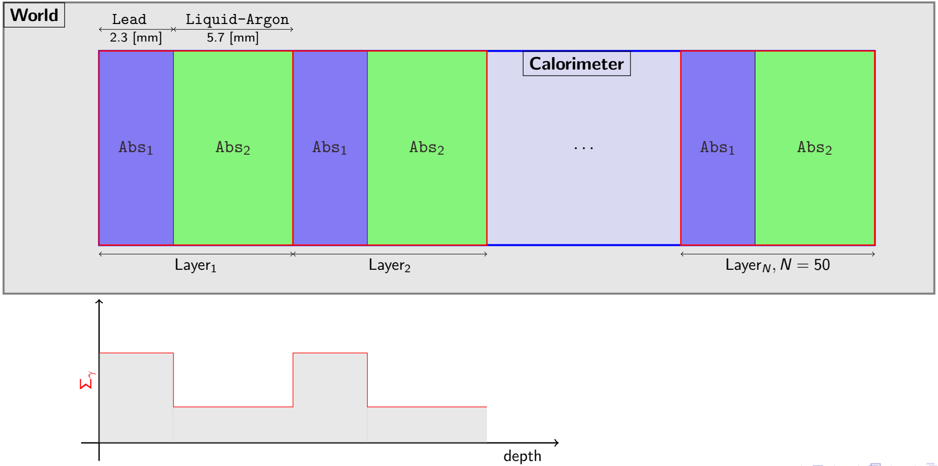

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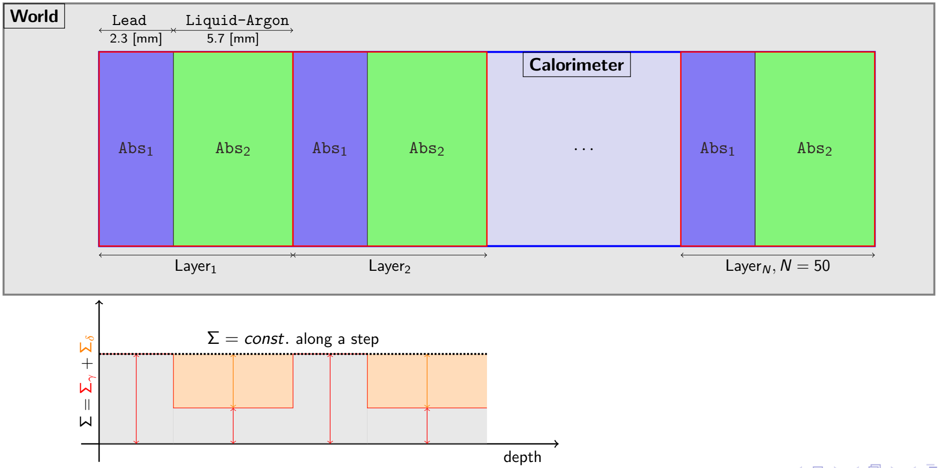

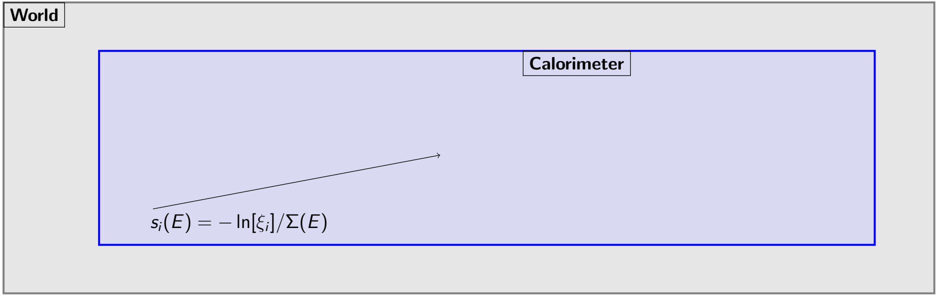

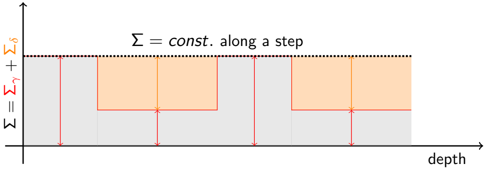

- $s(E) \sim \mathbb{E}\text{xp}\left[\Sigma(E)\right]$ with $\Sigma(E) = \max\{\Sigma_\gamma(E, \text{Abs}_i)\}$
- $s_i(E)$ might correspond to crossing several boundaries

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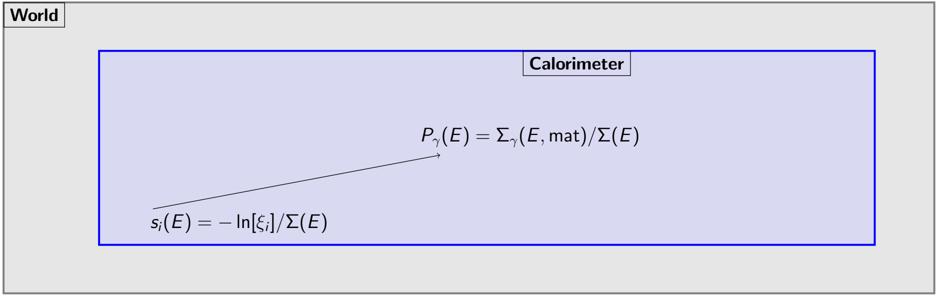

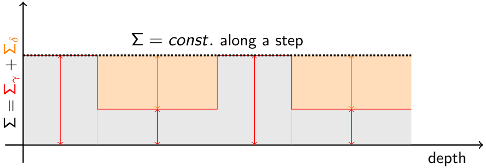

- $s(E) \sim \mathbb{E}\text{xp}\,[\Sigma(E)]$ with $\Sigma(E) = \max\{\Sigma_\gamma(E, \text{Abs}_i)\}$
- $s_i(E)$ might correspond to crossing several boundaries
- Interact with probability $P_\gamma(E) = \Sigma_\gamma(E, \text{mat})/\Sigma(E)$
- Several steps might be done without interaction ($E = const.$)

Woodcock tracking in GEANT4

Example

Mean values per event of some selected quantities when modelling 10^4, $E_0 = 10$ [GeV] e^- in a simplified sampling calorimeter (50 layers of [2.3 mm `Pb` + 5.7 mm `lAr`]).

		"Normal way"	`Gamma-general`	`Woodcock(+GG)`
E_{dep} [MeV]	`Pb`	7726.3	7725.9	7725.7
	`lAr`	2145.6	2145.9	2145.6
#secondary	γ	5215.7	5216.2	5215.4
	e^-	8963.3	8931.2	8928.5
	e^+	538.5	538.3	538.3
#steps	`charged`	36548.4	36522	36860.5
	`neutral`	**36963.4**	**36952.7**	**9600.8**
Rel. perf. gain		0	$\sim$ 5 [%]	$\sim$ 15 [%]

- Woodcock tracking active whenever a γ track is inside the Calorimeter and $E > 200$ keV

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Implementation

- `Woodcock` process derived from `G4GammaGeneralProcess`
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  - Additionally pass name of a region for Woodcock tracking

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Implementation

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- Process can be added exactly like `G4GammaGeneralProcess`
  - Additionally pass name of a region for Woodcock tracking
- Also experimented with specialized tracking (`G4VTrackingManager`)
  - Based on older version of process, not updated to latest improvements

Woodcock tracking in GEANT4

Summary & caveat

- Woodcock tracking can significantly reduce number of neutral steps
  - Up to factor 2x – 4x with observables in statistical agreement, but faster simulation
  - Preliminary results: up to 10 % overall improvement when applied to ATLAS EMEC

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Summary & caveat

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  - Up to factor 2x – 4x with observables in statistical agreement, but faster simulation
  - Preliminary results: up to 10 % overall improvement when applied to ATLAS EMEC
- **Breaks the important convention that tracks stop at volume boundaries!**
  - Implication: pre-step point in different volume than (discrete) interaction
  - Requires update of user codes (sensitive detector and stepping action)

Combining transportation and Multiple Scattering

Somewhat similar problem with charged particles (here: electron):

Step#	[...]	KineE	dEStep	StepLeng	TrakLeng	Volume	Process
0	[...]	10 MeV	0 eV	0 fm	0 fm	World	initStep
1	[...]	10 MeV	1.214e-15 meV	4 cm	4 cm	World	Transportation
2	[...]	9.469 MeV	530.7 keV	442.5 um	4.044 cm	G4_Pb	msc
3	[...]	8.78 MeV	689.5 keV	549.8 um	4.099 cm	G4_Pb	msc
4	[...]	8.167 MeV	612.5 keV	576.7 um	4.157 cm	G4_Pb	msc
5	[...]	7.287 MeV	678.7 keV	535.8 um	4.21 cm	G4_Pb	eBrem
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  - Must not make too long steps for approximations to remain valid
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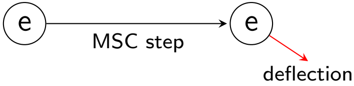

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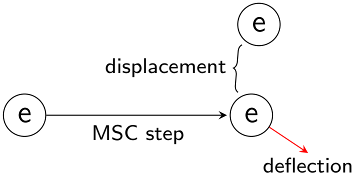

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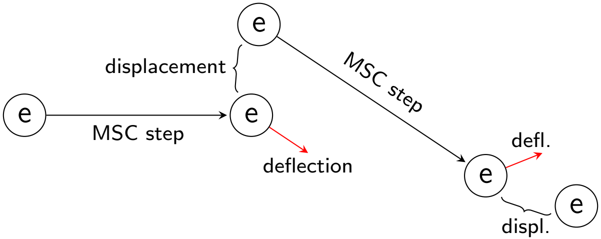

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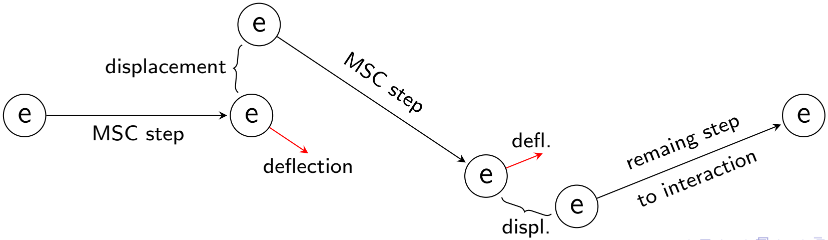

Combining transportation and Multiple Scattering

Implications

- At every "interaction point", GEANT4 must handle the machinery of a full step
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- Can we do better / be more efficient for the default settings?

Combining transportation and Multiple Scattering

G4TransportationWithMsc

- Combine transportation and MSC into one process: G4TransportationWithMsc
  - Inherit from G4Transportation for the actual transportation (linear or in field)
  - Implements code similar to G4VMultipleScattering that calls G4VMscModel

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  - Inherit from `G4Transportation` for the actual transportation (linear or in field)
  - Implements code similar to `G4VMultipleScattering` that calls `G4VMscModel`
- With `/process/em/transportationWithMsc Enabled` (since `ref-04`):
  - Identical results to using `G4VMultipleScattering` and `G4Transportation`
  - Tiny performance advantage with only one process / `G4VParticleChange`

- To solve the actual problem, take advantage of combined process:
    1. Receive the proposed (true) step length from other processes
    2. Determine MSC step limit & convert to geometric step length
    3. Transport track according to step length
    4. Apply MSC angular deflection and displacement
    5. If no boundary and step length left, go back to 2.
    6. Otherwise, track arrived at "true" interaction point

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- Added in `geant4-dev` for `ref-05`, available in `11.1-beta`
  - Enable with `/process/em/transportationWithMsc MultipleSteps`

- Saved work for internal steps:
  - Evaluation of cross sections (instead handled by "integral approach")
  - Energy loss fluctuations (mean energy loss still needed)
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- Testing with simplified sampling calorimeter (as before; replace lead by $PbWO_4$)
  - `opt0` EM physics, simulating 10^5 electrons at 10 GeV with 24 threads
  - Mean number of charged steps almost cut in half! (35975.5 $\to$ 18467.9)
  - Simulation time reduced by 16.5 % (524.5s $\to$ 437.6s)

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- Integrated into CMSSW and testing under way (no validation yet)
  - Little difference for Run3 geometry, bigger potential for Phase2 and HGCal
  - Preliminary results indicate $\approx 5\,\%$ improvement for `FTFP_BERT_EMM`, up to $20\,\%$ for `FTFP_BERT_EMN` with most precise GS settings

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  - Investigate computing performance improvements for EM shower generation
- Compact library of EM processes for HEP
  - Covers the complete physics for $e^{\pm}$ and γ particle transport
  - See source code on GitHub and the documentation
- See also previous presentations
  - last Collaboration Meeting
  - Technical Forum in March 2021

- Switched implementation of Multiple Scattering to Urban model
  - Facilitate experiment validation & eventual transition

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Changes since last Collaboration Meeting

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- Added energy loss fluctuations
  - Simplified model based on GEANT4 11.0

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  - Facilitate experiment validation & eventual transition
- Added energy loss fluctuations
  - Simplified model based on GEANT4 11.0
- Integrated specialized tracking manager with GEANT4 11.0
  - Including the internal MSC stepping presented in the previous part (active by default, but can be deactivated)

- ATLAS
  - Investigated differences in multiple scattering between GEANT4 10.6 and 11.0
  - After some work, passed pre-validation in Athena framework

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  - After some work, passed pre-validation in Athena framework
- CMS
  - Started testing integration with CMSSW
  - Identified some CMake problems, but prototype working in general
  - Not looked at results yet (neither performance nor validation)

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Summary

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- Presented two working prototypes for reducing number of steps
  - Woodcock tracking for γ, propagating across volume boundaries
  - Internal MSC stepping for charged particles (focus on $e^{\pm}$)

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- Presented two working prototypes for reducing number of steps
  - Woodcock tracking for γ, propagating across volume boundaries
  - Internal MSC stepping for charged particles (focus on $e^{\pm}$)
  - Both give results in statistical agreement, but faster!
- Working with simulation teams in ATLAS and CMS
  - Testing in realistic setups & with their requirements
  - Showing impressive gains for already well-optimized simulations