ATLAS Full Simulation Group
- Status Report -

Geant4 Technical Forum #60

Feb. 15, 2024

Dongwon Kim
on behalf of the ATLAS Full Simulation Group

ATLAS Full Simulation Group

GOAL: *Improving FullSim's performance without a significant loss in physics precision (with a close collaboration with Geant4 experts on various topics)*

List of Topics

1. Geant4 11
2. EMEC implementation
3. Test of ATLAS Calorimeter with Geant4 and FLUKA.CERN
4. Model Tuning on ATLAS data
5. Parameter Tuning of In-Field Tracking
6. Energy Loss Fluctuation

Other on-going activities (Back-up)

1. Voxel density optimisation
2. ISF particle killer
3. AdePT / Celeritas in FullSimLight

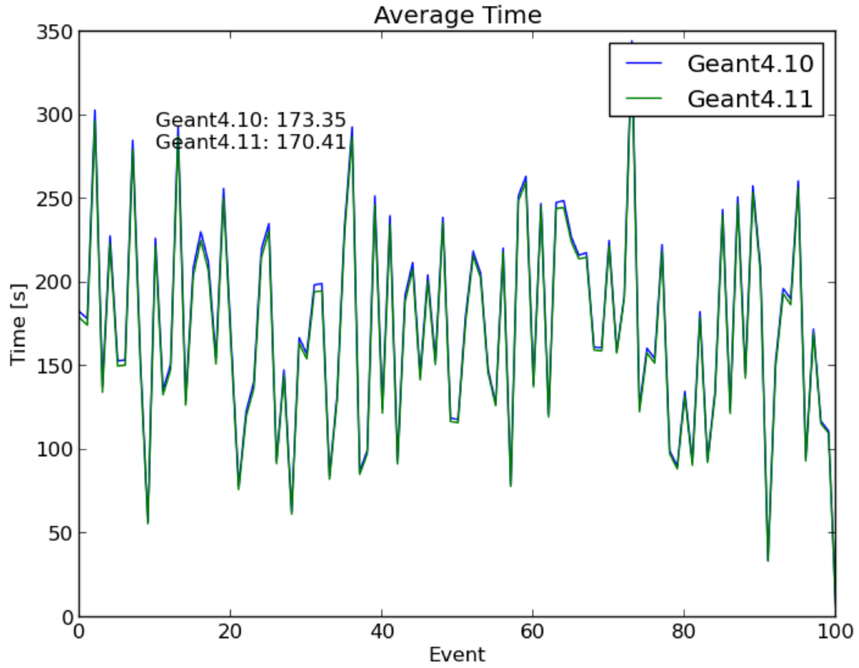
Overall Performances in ATLAS

Feedback to Geant4 Collaboration

- Topics in Geant4 Technical Forum #59:
  https://indico.cern.ch/event/1266537/timetable/?view=standard#23-atlas-geant4-simulation-upd

Geant4 11.1

- Implemented *geant4-11.1.3-atlaspatch-2* (only major difference related to Woodcock tracking added to *G4EMStandardPhysics*) into Athena using a private build (available in cvmfs)
- Physics validation ongoing
  - EM physics in Geant4 11.1 seems similar to 10.6 in physics performance plots, i.e. an order of per-mil changes in energy scale for electron and photon validation
- Working on streamlining the cycle for the adaptation of a new Geant4 version (physics validation, performance, calibration, sampling fractions)
- First benchmark results available
- A performance increase of ~ 1.7% (100 ttbar events)
- Next step: validation of Geant4 11.2.patch01

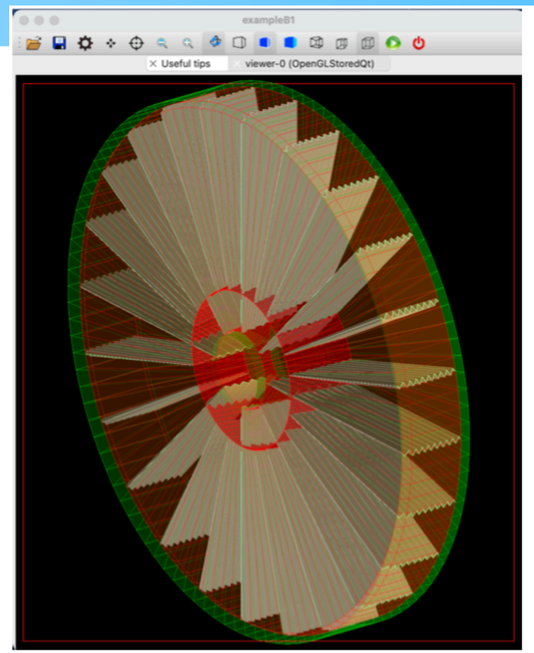


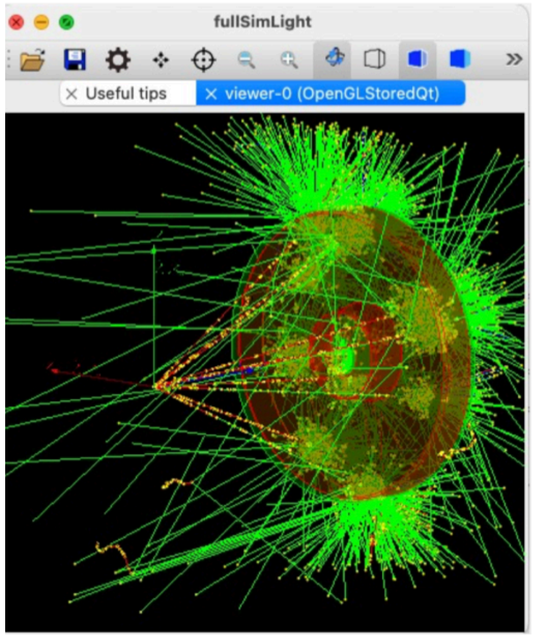
EMEC implementation (1)

Goal: Define the geometry of EMEC with Standard G4 / *VecGeom* shapes to fasten the simulation as well as allow the usage in other architectures such as GPU

- Speed up stemming from the "Custom solids → G4 solids" implementations
  - also, enables us to represent the geometry using *VecGeom* with GPUs

- **Status**:
  - A complete EMEC accordion structure is implemented both in a standalone Geant4 example and as a GeoModel plug-in
  - Implemented geometry consists of
    (1) EMEC mother volume
    (2) Inner/Outer Wheel envelopes
    (3) Inner/Outer Wheel Absorbers and Electrodes (defined as G4 GenericTrap solids)
  - Implementation is guided by the data found in the technical drawing of the lead plates for the Inner and Outer Wheel Absorbers (More details in BACK-UP)
  - Material definitions have been extracted from C++ code used in the HEC Test Beam





EMEC implementation (2)

Test Run Results with 10 GeV e^- with Geant4 11.2

- Current EMEC version with subdivisions into sectors

	Custom solid		G4GenericTrap, no slices		G4GenericTrap, slices		G4GenericTrap slices + sectors (16, 24)	
	Geant4	G4+VecGeom	Geant4	G4+VecGeom	Geant4	G4+VecGeom	Geant4	G4+VecGeom
CPU	100 s	90 s	42 (-9) s	29 (-4) s	33 (-9) s	25 (-5) s	42 s	29 s
Mean energy deposit per event [GeV]	9.917 +- 0.04767	9.915 +- 0.04781	9.907 +- 0.06408	9.907 +- 0.06023	9.913 +- 0.05428	9.869 +- 0.5478	9.908 +- 0.05606	9.895 +- 0.1997
Mean track length (charged) per event [cm]	2259 +- 167	2275 +- 177.2	2058 +- 161	2311 +- 183.4	2105 +- 216	2306 +- 220.9	2111 +- 210	2306 +- 191.1
Mean track length (neutral) per event [cm]	2.688e+04 +- 2395	2.726e+04 +- 2695	3.053e+04 +- 3031	2.78e+04 +- 2741	3.006e+04 +- 3308	2.716e+04 +- 3084	3.065e+04 +- 3346	2.73e+04 +- 2526
Number of steps (charged) per event	6.375e+04 +- 1036	6.371e+04 +- 1068	6.603e+04 +- 1366	5.305e+04 +- 950	6.675e+04 +- 1367	5.281e+04 +- 3041	6.737e+04 +- 1432	5.482e+04 +- 1435
Number of steps (neutral) per event	1.199e+05 +- 2936	1.197e+05 +- 3129	1.18e+05 +- 2916	1.199e+05 +- 3010	1.228e+05 +- 3297	1.223e+05 +- 7731	1.29e+05 +- 3755	1.296e+05 +- 4452
Number of secondaries per event :								
Gammas	4893 +- 66.65	4889 +- 65.5	4831 +- 74.08	4861 +- 304.8	4829 +- 74.97	4866 +- 283.8	4838 +- 75.51	4875 +- 118.2
Electrons	9127 +- 131.8	9114 +- 131.6	9873 +- 177.6	9066 +- 575.4	9878 +- 171.5	9080 +- 533.5	9894 +- 196	9092 +- 229.2
Positrons	485.4 +- 15.25	484.5 +- 15.36	469.1 +- 15.48	482.2 +- 33.28	471.8 +- 15.75	483.8 +- 31.5	472 +- 15.25	484.4 +- 19.2

- When compiled *FullSimLight* with *VecGeom*, the results changes each time one recompiles it, affecting the physics results.
- A use of *VecGeom UnplacedGenTrap* → many "stuck tracks", i.e. some event were aborted due to excessive numbers of zero traps.

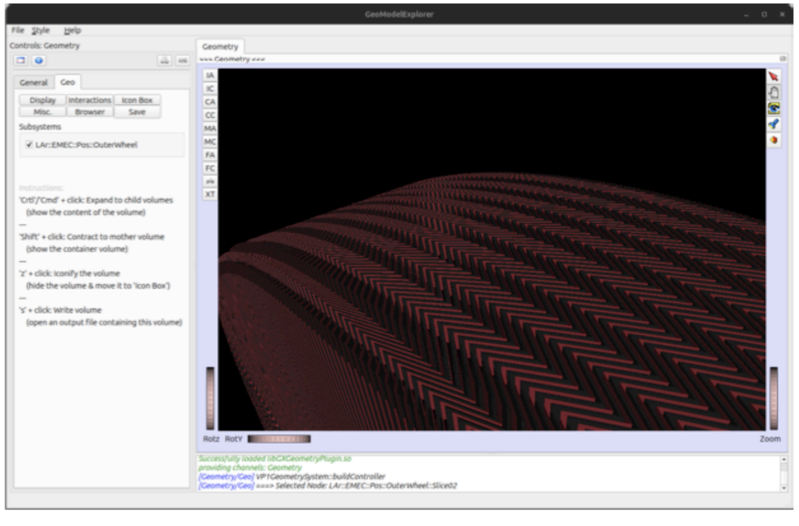
→ Both issues are under investigation

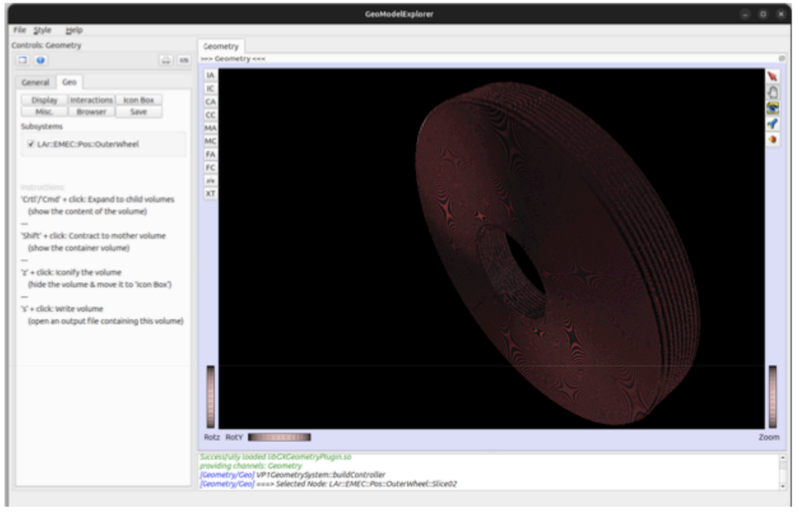
EMEC implementation (3)

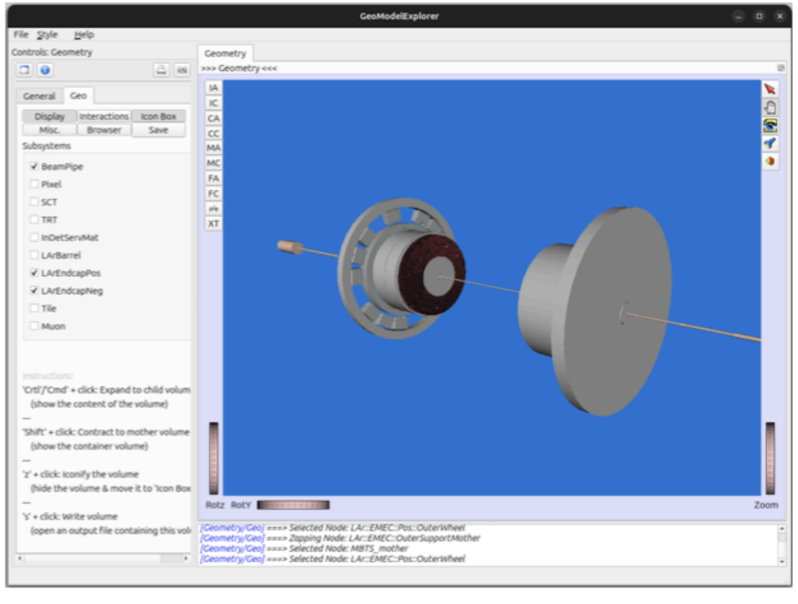
Evgueni Tcherniaev, Marilena Bandieramonte

GeoModel plug-in with new EMEC implementation

- Runs fine in *FullSimLight* (with all the *GeoModel* tools)
- First time the EMEC visualisation in *gmex* and other visualisation tools (e.g. *VP1*)
- An export of ATLAS geometry in *GDML* format is now possible
  - a support for G4DisplacedSolids in GDML parser would be really helpful (implemented a hack to circumvent the issue)
- Marilena B. succeeded in the code integration into Athena using private branch and currently running benchmarks for comparison: observed ~ 19% speed-up in total CPU time of an ATLAS simulation (500 ttbar events)
- Follow-up tasks:
  - need to fix a bug in *G4GenericTrap* both in Geant4 and VecGeom
  - run physics validation after solving the geometry bug





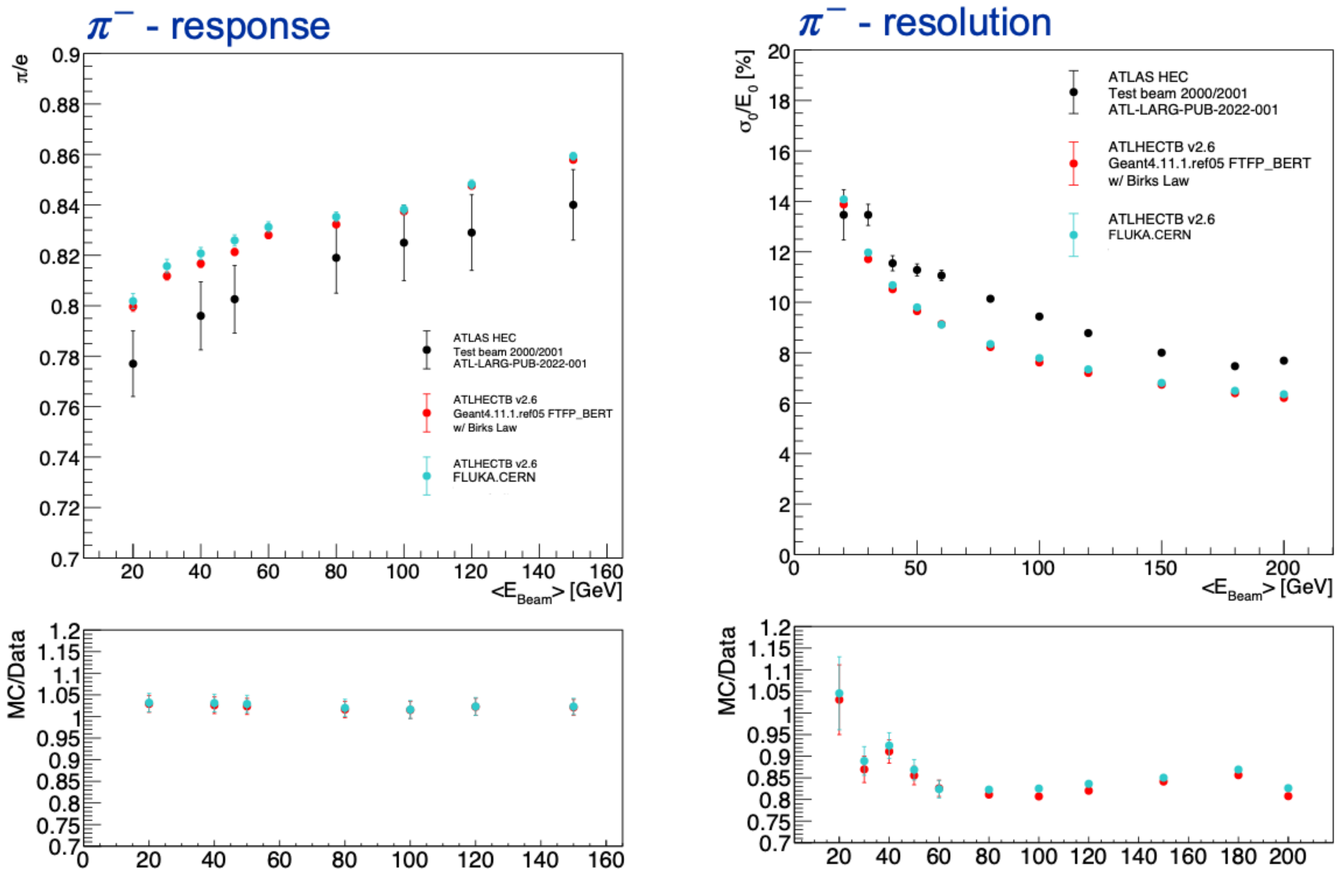


Testing ATLAS Calorimeter with GEANT4 and FLUKA.CERN

Goal: Check the performances of *FLUKA* hadronic event generator in *ATLAS* calorimeters (*HEC* / *TileCal*)

Status:

- The tests are performed with ATLAS *HEC* / *TileCal* beam-test setups.
- Several sanity checks on ATLAS *HEC* G4 vs. *FLUKA* have been performed: energy response, resolutions, barycenter longitudinal position, and shower length (also, for *TileCal*)



- For the case of *HEC*, Geant4 11.1 and *FLUKA.CERN* are in a good agreement, but have a discrepancy with the data.
- For the case of *TileCal*, Geant4 shows a better agreement with the data compared to *FLUKA.CERN* in energy response and resolution.
- Further investigation is ongoing to comprehend the issues in detail.

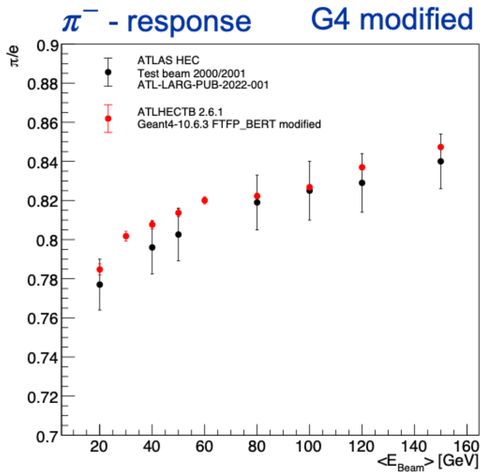
Source: Presentation by L.Pezzotti

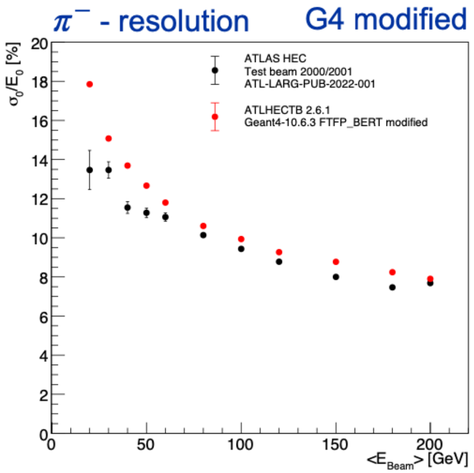
Further Model Tuning on ATLAS data

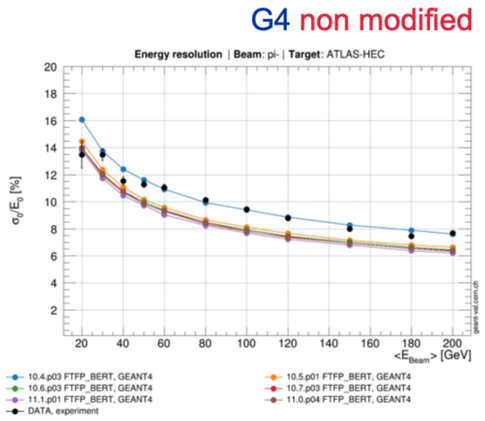
Goal: Retrieve ATLAS energy resolutions with newer version of Geant4

Status:

- Run 3 MC Campaign: Geant4 10.6 (too narrow signal fluctuations)
- Adjust the FTF parameters (*G4FTFParameters.cc*) - affects charge-exchange string-formation process + nuclear destruction
  - increase the probability of having a change-exchange process during the string formation
  - increase the probability of involving a neighbouring nucleon during the Reggeon cascade
  - increase the excitation energy per wounded nucleon
- Only affect $\pi^{\pm}$-induced showers







- Modified FTFParameters lead to a better agreement in the response (π/e), within ATLAS error bars (same for TileCal)
- Further optimisation for matching the ATLAS data is ongoing.

Source: Presentation by L.Pezzotti

Parameter Tuning of In-Field Tracking

Goal: Find the optimal values of the in-field tracking parameters for physics performance and CPU savings

- The study is motivated by the tuning performed by CMS (for full simulation for Run 3)
- Lists of tuning parameters + descriptions for tracking in a magnetic field

  - DeltaIntersection: accuracy of intersection with boundary volume

  - DeltaOneStep: accuracy for endpoint of 'ordinary' integration step

  - DeltaChord: approximation of curve with linear sections

  - MaxStep: maximum step length
- The tuning can be done for different detector regions and various particle energies

Status:

- Currently, working on the implementation of a *G4FieldManager* derived class in FullSimLight to be able to control those parameters by filtering on the particle energy and the geometry
- Next step: perform parameter optimisations for the complete geometry, using the parameter sets specified by CMS, for 100k events
- For the detector specific region tracking, the study for the tracker and other regions will be conducted soon, upon implementation of the settings

Energy Loss Fluctuation

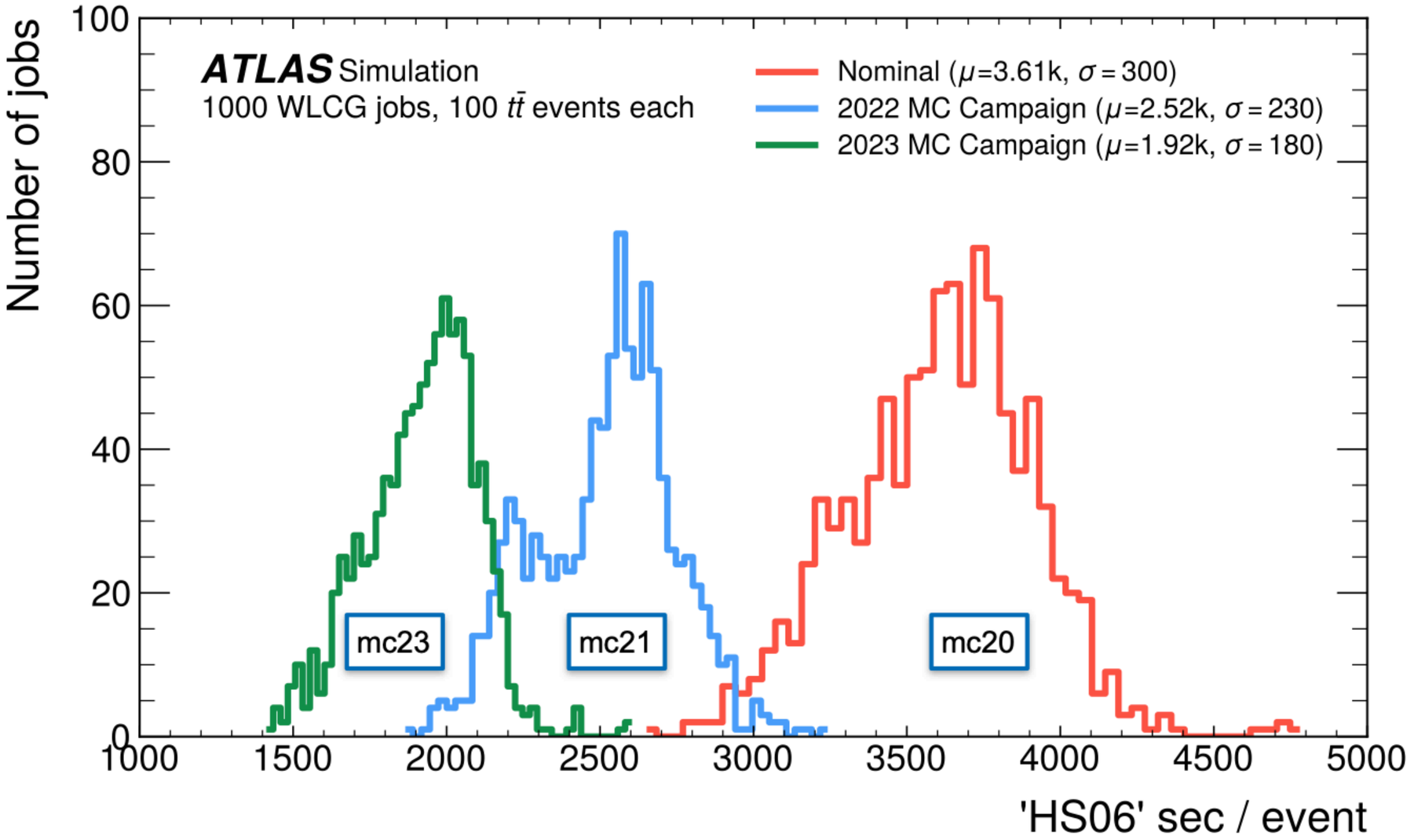
Goal: Test the performance gain of switching off the energy loss fluctuation in Geant4.

- If a substantial CPU gain exists, go for physics validation for checking physics accuracy.

Approach:

- Can be done using the Geant4 command */process/eLoss/fluct false*
- First to be performed in FullSimLight and then in Athena

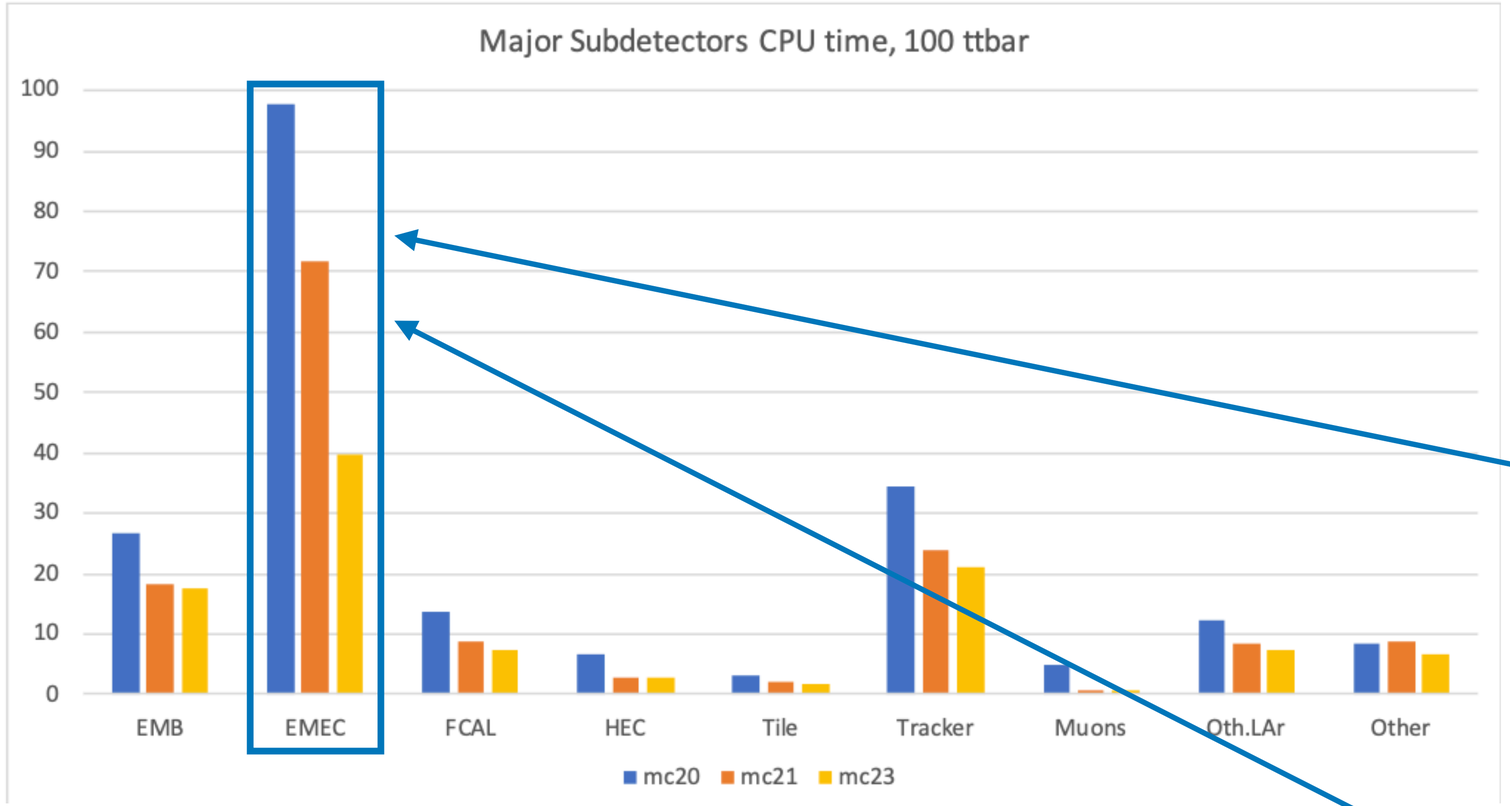
Performances of ATLAS Simulation



- Run 3 simulation ~ × 2 faster than Run 2 !!

Source: 28th Geant4 Collaboration Meeting

Improvements over different MC campaigns



- mc20, MC reprocessing campaign for Run2
  - TRT range cut (for e-/e+)
  - Frozen showers
- mc21a, MC campaign for start of Run3 (+mc20)
  - EM range cuts
  - PRR, NRR
  - EMEC slices
  - Big Library
  - MagField Off
  - G4GammaGeneralProcess
  - BeamPipe killer (kills particles at eta > 5.5)
- mc23c (+mc21), MC campaign for Run3
  - Woodcock tracking (for gammas)
  - VecGeom (usage of Polycons, Tubes, Cones)

- EMEC is the dominant contribution to ATLAS Full Simulation
  - EMEC > Inner detector (Tracker) > EMB
- In mc23c, a clear reduction of time spent in the EMEC
- Link Time Optimisation (LTO): 4% speed up in Athena/FullSimLight (Ben Morgan)

→ aim to implement this in 2024 MC Campaign

Source: 28th Geant4 Collaboration Meeting

Feedback to Geant4 Collaboration

Physics:

- A close collaboration with Geant4 experts has led to the implementations of new improvements and fixes, particularly in areas such as EM physics, Woodcock tracking, Voxel density, etc.
- A significant improvement in CPU consumptions with a good physics accuracy is observed in different MC campaigns and sub-detectors, esp. in EMEC (See previous Benchmark slides)
- We look forward to having the possibility to fully integrate *G4HepEM* (development needed on the G4 side to enable all the optimisations, i.e. Woodcock tracking and *G4GammaGeneral* process) and test the custom tracking manager, combined transportation, and multiple scattering.
- We look forward to continuing this collaboration on future projects!!!

R&D:

- Developments related to GPU workflows (e.g. Celeritas and AdePT) are on-going and ready to test some benchmarks / validation.

Thank you for your attention!

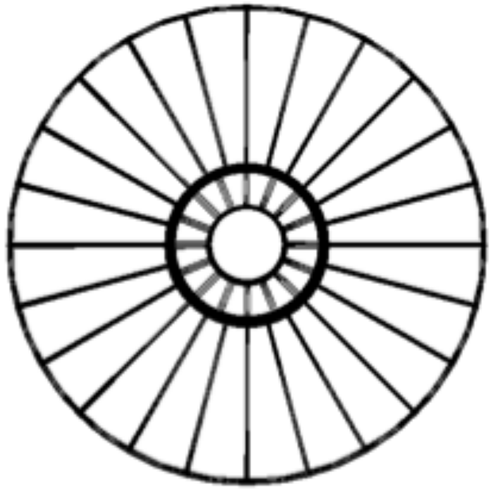
Backup

EMEC implementation

Technical Drawing of the lead plates for the Inner / Outer Wheel Absorbers

- The option to divide EMEC wheels into sectors has been incorporated into the EMECAccordionConstruction class
- Each sector is constructed as a Boolean intersection of G4Cons and G4GenericTrap
- An application of subdivision into sectors decreases the performance

→ A possible solution: subdivision into slices as GEANT4 voxelisation does not need further assistance.



Voxel Density Optimisation

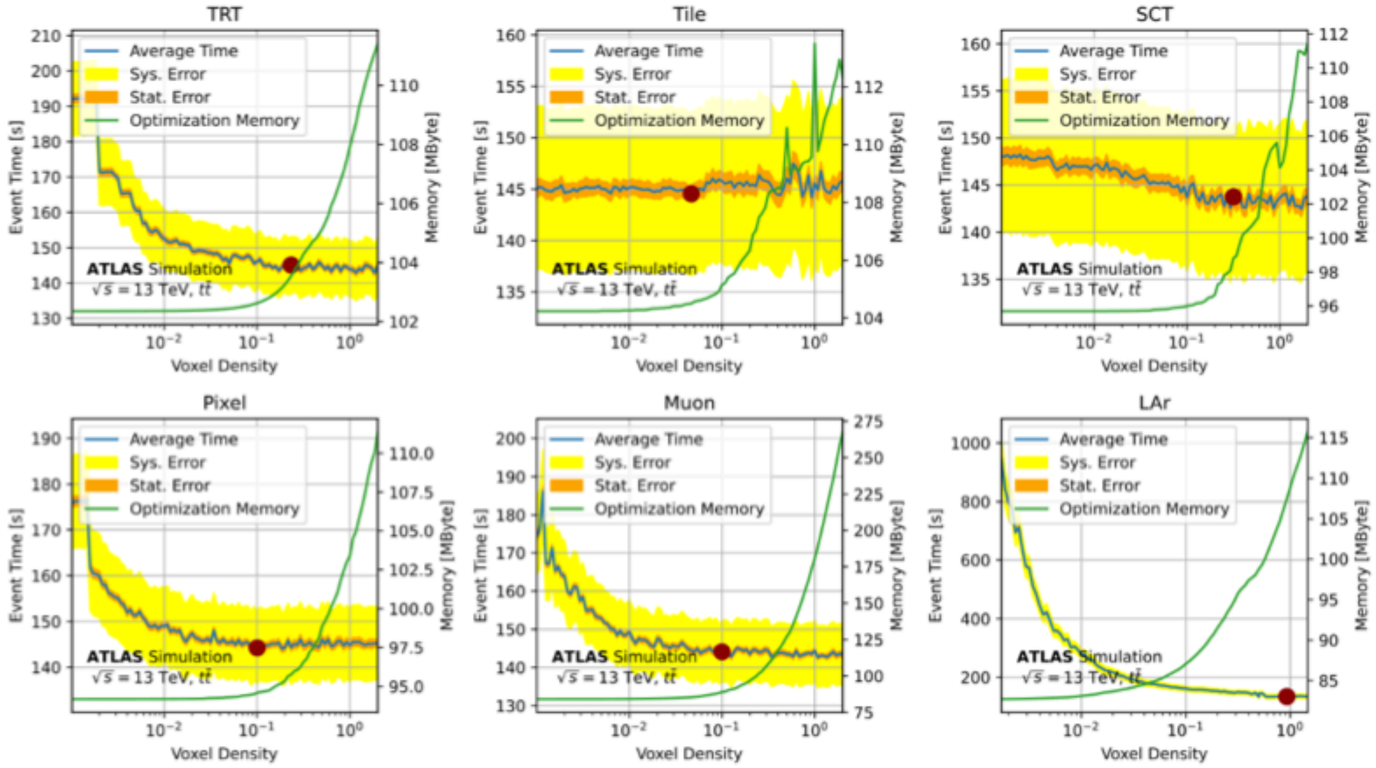
Goal: Find optimal values of voxel densities in Run-3 geometry

- Tune the voxel size and granularity via "smartless" GEANT4 parameter for optimal memory and CPU consumption.

Status:

- Studied changes in standalone simulation frame work (FullSimLight) and Athena
  - Improvement in memory consumption for geometry optimisation
  - Completed physics validation
  - Observed an increase of CPU consumption

  → Follow-up studies are on-going



High-η particle rejection (ISF Particle Killer)

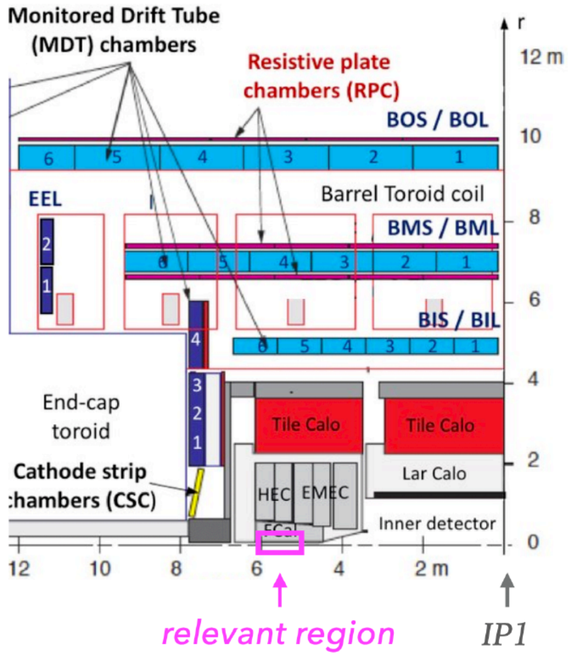
Goal: Kill primary particles generating secondaries close to the beam-pipe at 5 ~ 6 m

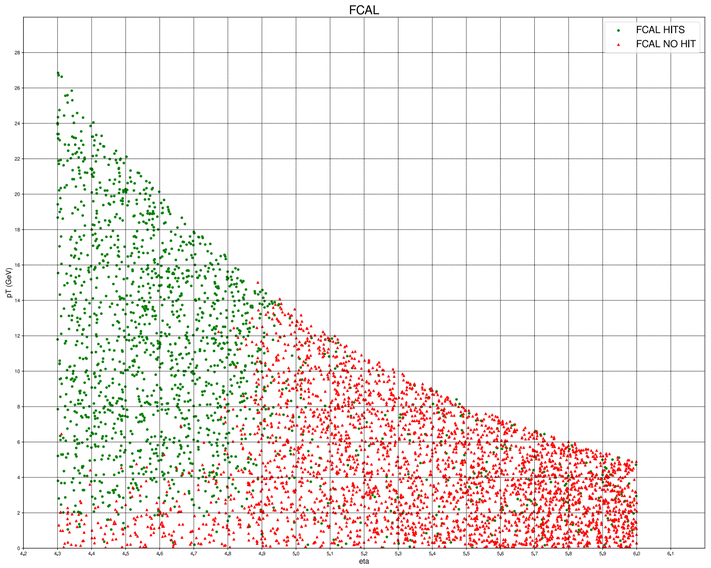
- Many particles in the collision are at high $|\eta|$ (no ID hits) with little energy compared to the calorimeter noise.
- Check if we can kill some particles early on which will have no or little effect on the simulated energy in the calorimeters to save CPU.

Status:

- 2d map (p_T vs. η) is obtained
- Technical studies on how to classify particles as significant or not are on-ongoing
- Not clear where to make a cut as there are some cases that still provide cluster energy deposits
- Require more benchmark points to decide the importance of event
- Perhaps, look for a clear border that we can "safely" ignore particles

  → run physics validation with newly chosen border





AdePT / Celeritas in FullSimLight / TileCal

Goal: Use GPU for ATLAS simulation

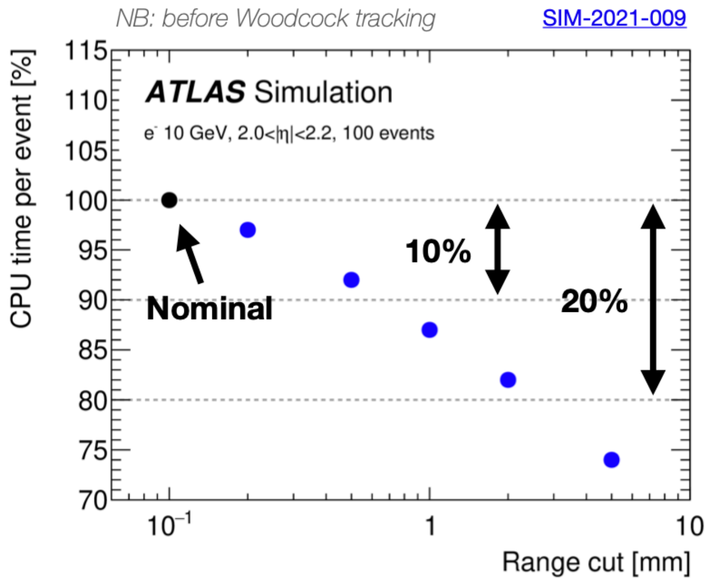
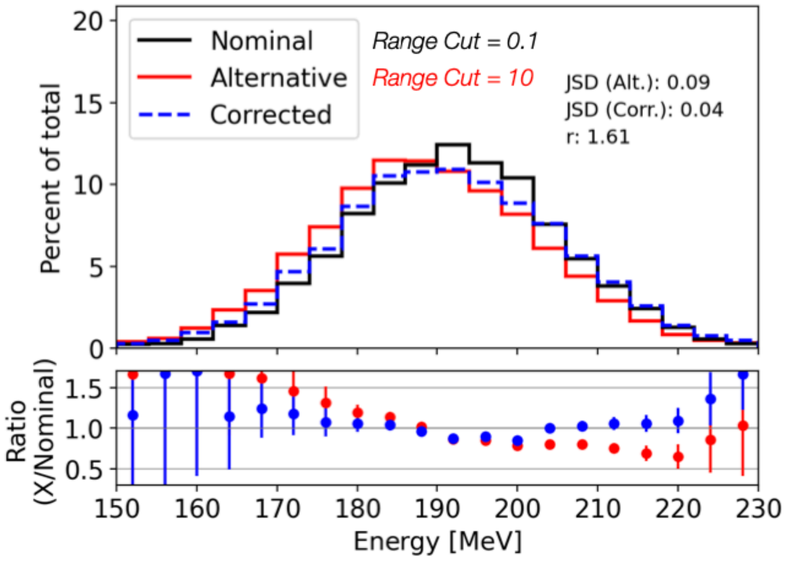
Status:

- Recent AdePT & Celeritas meeting (Dec. 10 -15, 2023): more synergies between the projects
- New test tools for benchmark and validation available (J.G. Caminero)

Integration with ATLAS:

- Initial work done for integrating **Celeritas** offload/transport in the Tile calorimeter test beam simulation validation application:
  - https://github.com/celeritas-project/atlas-tilecal-integration
  - From: https://github.com/lopezzot/ATLTileCalTB
  - Runnable through FullSimLight as a plugin, although currently built using a fork of GeoModel: https://github.com/celeritas-project/GeoModel
- **AdePT** example of the Tile calorimeter test beam simulation implemented by Davide:
  - Now beginning work to implement this as a FullSimLight plugin as has been done for **Celeritas**
  - https://indico.cern.ch/event/1215829/contributions/5306569/

ML correction for range cut configuration

Goal: use ML to make aggressive range cuts (i.e. higher range cuts)

- Increased range cuts can reduce number of particles / simulation steps while increasing the computation performance
- Range cuts can be applied globally or different detector regions
- *High* range cuts may lead to a loss in physics precision
- Approach:
  - simplified calorimeter rewriter: use classification NN (3D CNN) to approximate likelihood-ratio test
  - train on cell-level energy deposits
  - invert likelihood-ratio to get weights
  - Re-weight experimental observables
- Drawbacks:
  - weights introduce biased simulation paradigm (contrast to the analog ATLAS currently use)
  - weights induce statistical dilution
  - Irregular ATLAS calorimeter segmentation as well as energy deposits prohibits direct convolution operations