Update on Geant4

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10 years of development : G4 9.6 – 11.0

Geant4 **9.6** (2012)

- Several extensions and improvements of BERT model
  - Changed internal nucleon-nucleon cross sections
  - Extended to gamma-nuclear interactions
  - Extended to nuclear capture at rest
- Replacement of CHIPS with FTFP and BERT models
  - For gamma-nuclear and lepton-nuclear
  - For nuclear capture at rest
- INCLXX (alternative, precise intra-nuclear cascade model)
  - For pions, nucleons and light ions projectiles
  - From ~100 MeV up to ~3 GeV
  - Available in the physics list QGSP_INCLXX

Geant4 **10.0** (2013)

- Improved neutron capture (without NeutronHP)
  - FTFP_BERT becomes closer to FTFP_BERT_HP
  - Strongest effect for Tungsten
- Further improvements of BERT
  - 2-body angular distribution
  - Phase-space generation for multi-body final states
- Extended Fritiof (FTF) string model to nucleus-nucleus
- Removed CHIPS and parametrized (Gheisha-like) models
  - Replaced by FTFP and BERT (already in G4 9.6)
- Extensions of reference physics lists
  - All EM variants (*e.g.* _EMZ) available through G4PhysListFactory
  - Various INCLXX possibilities: FTFP_INCLXX, QGSP_INCLXX_HP, *etc.*

Geant4 **10.1** (2014)

- Thin-target improvements of Fritiof (FTF) string model
  - Minor impact on hadronic showers
- Improved string fragmentation of Quark Gluon String (QGS)
  - Large effect on hadronic showers
    - Lower energy response and bigger (wider and longer) showers
- INCLXX extended up to 20 GeV
  - INCLXX-based physics lists use FTF or QGS above 15 GeV
- Others
  - Switched on muon-nuclear by default in all physics lists
  - For physics lists with NeutronHP, set to zero the cut on proton
    - To simulate all nuclear recoils from elastic scattering

Geant4 **10.2** (2015)

- Improved treatment of excited nuclear remnants in FTF model
  - Affecting the production of low-energy protons and neutrons
    - Improved thin-target agreement, few percent increase in energy response of hadronic showers
- Important fix in inelastic and capture neutron cross sections
  - Affecting the lateral shapes (narrowing) of hadronic showers
    - FTFP_BERT and FTFP_BERT_HP getting closer
- Improved gamma emissions by nuclear de-excitation
- Improved energy conservation in radioactive decays
- ParticleHP
  - Include NeutronHP (precise transportation of neutrons below 20 MeV)
  - Extension for proton, deuteron, triton, He3 and alpha below 200 MeV
    - New data set G4TENDL based on ENDF and TALYS
    - Used only in QGSP_BIC_AllHP

Geant4 **10.3** (2016)

- Improved evaporation spectrum of BERT model
  - Reduced over-production of low-energy neutrons and protons
- Changed transition energy between FTFP and BERT
  - From **[4, 5]** GeV to **[3, 12]** GeV – for pions, kaons, and nucleons
- Not released developments in FTF and QGS string models
  - Improved thin-target description but worse hadronic showers
    - *E.g.* higher energy response and narrower showers
  - Motivated by the need of the LHC experiments to have stable simulation of hadronic showers during Run 2
    - Important for the simulation of jets
  - Released so-called “stable/production” version of string models, developments available in the beta release, 10.3.beta

Geant4 **10.4** (2017)

- EM Opt4 (_**EMZ**) has state-of-the-art multiple scattering
  - **Goudsmit-Saunderson (GS) model with Mott correction**
- Extended INCLXX to the strangeness sector
  - Handling of kaons and hyperons projectiles, and production of secondary kaons and hyperons
- New combined (LEND+BERT) gamma-nuclear model
  - Use LEND data for gammas below 20 MeV if available, BERT for the rest
- Enabled production and transport of long-lived isomers
  - Before (and now for isomers below a time threshold), force prompt decay to ground state
- New, experimental physics list FTFQGSP_BERT
  - FTF-based string formation and QGS-based string fragmentation
- Not released developments in FTF and QGS string models
  - Improved thin-target description but worse (higher) energy response in showers
  - Released so-called stable/production version of string models to keep stable hadronic showers
  - Developments available in the beta release, 10.4.beta

Geant4 **10.5** (2018)

- Revised gamma conversion and electron/positron bremsstrahlung models
  - Improved screening function, LPM effect, angular generation, and sampling efficiency
    - Better EM lateral shower shapes
- Released **new version of FTF and QGS** string models
  - Developed since the last three years (i.e. after G4 10.2) and kept on hold to guarantee stable hadronic showers for ATLAS and CMS
  - Better thin-target description, wider hadronic showers, but few percent higher response and smaller energy fluctuations in hadronic showers
    - Also few percent higher energy response in EM showers, due to improved back-scattering treatment in Urban multiple scattering model (which becomes closer to GS model and data)
  - New Birks quenching treatment recommended
    - Fit Birks coefficient from π/e test-beam data
  - QGS model becomes competitive with FTF above ~20 GeV
- Extended strange pair production channels in BERT model
- Consolidation of INCLXX model

Geant4 **10.6** (2019)

- Improved hadronic cross sections
  - Revised all hadron-nucleon cross sections at low energies
  - Extended Glauber-Gribov cross sections for hyperons and anti-hyperons
  - Gheisha-like cross sections are not used any longer
- Changed transition energy between string and cascade models
  - From **[3, 12]** GeV to **[3, 6]** GeV *(transiton between FTF and QGS unchanged: [12, 25] GeV)*
  - Consistently for all projectile particle types
    - Not only for charged pions, kaons, and nucleons: also for hyperons (instead of [2, 6] GeV), ions (instead of [2, 4] GeV/nucleons), and gammas (instead of [3, 3.5] GeV)
  - Not for FTFP_BERT_ATL, FTFP_INCLXX, QGSP_INCLXX, NuBeam, ShieldingM
- Validation and refinement of nucleus-nucleus modeling in FTF
- Added Radioactive Decay to all HP-based physics lists
  - This was already the case only for Shielding, LBE, QGSP_BIC_HP, QGSP_BIC_AllHP
- New neutron data library G4NDL**4.6**
  - Mostly based on JEFF-3.3 : more isotopes and better agreement with MCNP

Geant4 **10.7** (2020)

- Included **charm and bottom hadron nuclear interactions**
  - EM interactions (ionization & multiple scattering) already present before
  - Extension in: hadronic (elastic and inelastic) cross sections, elastic scattering, and string models (FTF and QGS)
    - Simplified decay treatment; no cascade model: FTF used down to 100 MeV, and below simplified treatment; usual transition between FTF and QGS : [12, 25] GeV
- Extended usage of QGS in QGS-based physics lists
  - For hyperons, anti-hyperons, anti-proton and anti-neutron above 12 GeV
- New gamma-nuclear final-state model below 200 MeV
  - Based on pre-compound de-excitation (BERT used above 199 MeV)
    - G4LowEGammaNuclearModel : can produce isomers and gamma transitions
- Optional scaling factors for elastic and inelastic hadronic cross sections
  - For studies of systematic uncertainties
    - 3 categories of hadrons: nucleons, charged pions, all others

Geant4 **11.0** (2021)

- Opportunities of a new major release
  - Removed old classes (*e.g.* Gheisha cross sections, old ion cross sections, old utilities), old interfaces, old UI commands, *etc.*
  - Replaced old, deprecated environmental variables used in ParticleHP with corresponding new UI commands
- Major improvement in the treatment of thermal neutrons in ParticleHP
  - Neutrons with E_{kin} < 4 eV – solved long-standing disagreement with MCNP
- New gamma-nuclear cross section
  - Better treatment of the Giant Dipole Resonance region (0-130 MeV)
    - G4GammaNuclearXS, based on IAEA evaluated photo-nuclear library
- New cut to kill very late radioactive decays at rest
  - Decays happening later than a time-threshold (default: 10^27 ns)
    - To prevent energy depositions happening after billions of years in ordinary materials used in calorimetry such as W and Pb, due to natural, unstable but long-lived isotopes such as W183, W180, and Pb204

Geant4 Versions
and
Physics Validation

Recommended Geant4 Version

- The recommended version is the latest, public release: as of today, Geant4 **11.0.p01**
  - Take advantage, at least, of the latest bug fixes and speed-ups
    - Typically a few percent with respect to the previous version
  - Moreover, latest developments in physics models
    - Often (but not always) improving the physics accuracy of the simulation, *e.g.* treatment of thermal neutrons
- Besides G4 11.0, we are still supporting the G4 10.7 series, with **10.7.p03** the latest patch available
- We are no longer fixing bugs for G4 **10.6** and earlier versions!
- Minor versions, **11.**{**1**, **2**, *etc.*} expected in the next few years
  - December releases + patches of recent releases

Physics Validation

- The physics validation of Geant4 – as done by CALICE and the LHC experiments – provides a snapshot of the accuracy of physics models for a given version of Geant4
  - A fundamental feedback for the models' developers
  - In general, the smaller is the gap between the version of a model that has been validated and its current (development) version, the more useful it is for its developers
  - Even more useful would be to re-run the validation for variations of a given model − *e.g.* including new effects, changing algorithms, or modifying parameters, *etc.* − well before a new Geant4 release
    - Keep in mind that Geant4 is used in production by several experiments, therefore it is not possible to make "explorative changes" in public releases...

==> One of the main benefits of porting validations in **geant-val** !

Physics Lists for HEP

Recommended Physics List for HEP: **FTFP_BERT**

- Used (eventually with variants) by the four big LHC experiments
  - ALICE uses FTFP_BERT, with **INCLXX** in the Tracker region
    - To get better production (with respect to BERT) of light ions in the beam pipe and inner tracker region via spallation by primary hadrons (pions and nucleons)
      - Using FTFP_INCLXX would cost a factor of 2 slow down in the simulation
      - It is possible to get "hadronic-model per region" by using generic biasing (see *examples/extended/hadronic/Hadr08/*)
  - ATLAS uses FTFP_BERT_**ATL**
    - Transition energy between FTFP and BERT in **[9, 12]** GeV
      - For charged pions, kaons, protons and neutrons – introduced in G4 10.2
  - CMS uses FTFP_BERT
    - With energy transition for charged **pions** in **[3, 12]** GeV
    - For all other particle types, standard transition [3, 6] GeV
  - LHCb uses plain FTFP_BERT

Tuning of Birks coefficient

- For scintillator-based calorimeters, the coefficient used for Birks quenching was obtained from old measurements, by fitting under the assumption of no delta-ray emissions
  - *i.e.* assuming that “energy loss” == “local deposited energy”
- This implies that the ionization density, dE/dx, was overestimated, and therefore the Birks coefficient was underestimated
- So, in realistic simulations where delta-rays are emitted, a higher Birks coefficient – and therefore a stronger quenching – should be applied, which implies smaller visible energy
- We suggest to **fit** the Birks coefficient by imposing the **π/e ratio** in simulation to be the same as measured in test-beam
  - ~ +50% in ATLAS TileCal (Fe-Sci), ~ +20% in ATLAS HEC (Cu-LAr)
  - ~ +15% in CMS HCAL (Cu-Sci)

“_**HP**” and “_**EMZ**” Variants

- FTFP_BERT_**HP** allows to evaluate how much the results depend on precise transportation of low-energy neutrons
  - Neutrons with kinetic energy below 20 MeV
  - With a significant slow-down of the simulation speed
  - Worth trying out at least for scintillator-based calorimeters
- FTFP_BERT_**EMZ** allows to evaluate how much the results depend on the most precise treatment of electromagnetic physics in Geant4
  - Recommended EM option for medical physics and space science
    - In particular, it has a state-of-the-art multiple scattering treatment (GS model + Mott correction)
  - With a significant slow-down of the simulation speed
  - Worth trying out for very granular calorimeters and/or gas-based calorimeters
    - It can affect the energy response and/or the lateral shape of electromagnetic showers

Hadronic String models: QGS *vs.* FTF

- In recent versions of Geant4 (10.6, 10.7, 11.0), QGS model becomes competitive with respect to FTF above ~20 GeV
  - In QGSP_BERT physics list, we use: FTF below 25 GeV
    QGS above 12 GeV

Reminder: QGSP_BERT was the physics lists used by the LHC experiments during the Run 1 (e.g. for the Higgs discovery); FTFP_BERT started to be used during the Run 2

- Hadronic showers: QGSP_BERT *vs.* FTFP_BERT
  - Few percent higher energy response
  - Wider energy fluctuation and worse (less optimistic) energy resolution
  - Few percent longer showers
  - 5-10% narrower showers

Hadronic Shower Simulations

Thin Target *vs.* Hadronic Showers

- Until Geant4 version 9.6, progress at thin-target level translated directly into progress in the simulation of hadronic showers
  - Reduced use of parametrized (Gheisha-like) model
  - Thorough revision of the Fritiof (FTF) string model
  - Improvements of Bertini (BERT) intra-nuclear cascade model
- With the Geant4 version 10.x series, progress at thin-target level produced often hadronic showers in tension with test-beam data
  - In particular regarding the energy response: developments pushed this quantity to increase, while test-beam data favoured lower values…
    - Even replacing BERT with more precise intra-nuclear cascade models, such as BIC or INCLXX, pushes towards higher energy responses in hadronic showers...
  - Some developments also caused the simulated hadronic showers to be narrower, whereas test-beam data favoured wider showers...

Why Tension between Thin- *vs.* Thick-target ?

- Various possibilities – including a combination of them
  - Thin-target improvements in some phase space regions – where we look or pay more attention – but perhaps worsening in others which might be important for hadronic showers
  - Thin-target data are richer in light materials (*e.g.* Be, C, Al, Si), whereas heavier materials (*e.g.* Fe, Cu, W, Pb) are more important for calorimetry
  - Current hadronic models might approach their ultimate physics accuracy capabilities – simplified, approximated treatments, not derived from QCD
  - Too naive tunings of hadronic model parameters – done mostly one parameter at the time, neglecting correlations
  - Incorrect Birks quenching
  - ...

Future Directions

- Enrich as much as possible the set of **thin-target data**, as well as the set of **calorimeter test-beams data** in ***geant-val***
- Better tuning of **FTF model parameters**
  - Correlated variations (*e.g.* using tools like Professor), different set of parameters according to particle type and/or particle energy, *etc.*
- Explore the best combination of the 3 intra-nuclear cascade models – **BERT** , **BIC** , **INCLXX** – in physics lists
  - Energy response seems the main difficulty to overcome...
- Optimize energy transitions between hadronic models
- Continue the development and refinement of physics models
- Synergies with the FLUKA-Cern group

Other Geant4-related Activities

HL-LHC Simulation Challenges

- HL-LHC experiments will need better (*i.e.* more accurate) and larger simulation samples than ever before
  - Else systematic errors will dominate
- The simulation of electromagnetic showers in calorimeters take a large fraction of the computing resources of experiments
  - Even hadronic showers are dominated by their EM component
    - From the decays of neutral pions into two gammas
- Large effort to speed-up simulations
  - Looking at electromagnetic physics, transportation, and geometry
    - Hadronic physics is **not** a leading player for CPU performance !
  - Goal: full (high fidelity) simulations as fast as possible, and fast (low fidelity) simulations as accurate as possible

On-going Activities

- Improvements and Optimizations
  - Model refinements, code revisions, better algorithms, more efficient memory layout, *etc.*
    - G4HepEm, Gamma General process, Woodcock tracking, DPM-like approach, *etc.*
- Fast Simulation
  - Improve and extend traditional HEP techniques
    - Shower parameterizations and shower libraries
  - Machine Learning generation of showers
- R&D on Accelerators and new Architectures
  - GeantV
  - AdePT and Celeritas : GPU prototypes for realistic EM shower simulations
    - Community meeting 3-6 May: https://indico.cern.ch/event/1123314/

Conclusions

Summary and Outlook

- Progress in Geant4 is continuing… but it is a bumpy road!
- Precise, reliable validation data is paramount
  - CALICE plays an important role here! Thanks a lot for your contributions!
- Three main challenges
  - More accurate physics simulations
    - Some physics analyses need the best detailed simulations; for others, faster, lower-fidelity approaches would suffice if similar enough to high-fidelity simulations
    - Even fast simulation needs full simulation samples for tuning / training
  - Faster simulations
    - Full simulation as much as possible, fast simulation as much as needed
    - Efficient use of available computing resources
  - Finding, training and **keeping** a new generation of developers
    - Many key developers of Geant4 are getting old...