

Geant4 - kernel updates

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Contents

- General introduction and brief
 updates of Geant4
- What's new in version 10
- New areas of user applications
- Near-future developments
- Geant4 the future





General introduction and brief updates







Geant4 History

R&D phase RD44)

Production phase

- Early discussions, for example at CHEP 1994 @ San Francisco
- Dec '94 R&D project start
- Apr '97 First alpha release
- Jul '98 First beta release
- Dec '98 First Geant4 public release version 1.0
- Several major architectural revisions
 - E.g. STL migration, "cuts per region", parallel worlds, multithreading
- Dec 8th, '17 Geant4 version 10.4 release
 - May 25th, '18 Geant4 10.4-patch02 release **Current version**
- We currently provide one public release every year.
 - Dec 7th, '18 Geant4 10.5 release Scheduled next release



Geant4 kernel update - M. Asai (SLAC)

10.4 came with new user's guides and new logo



Physics Reference Manual

Release 10.4

- The release in 2013 was a major release.
 - Geant4 version 10 release date : Dec. 6, 2013
- The highlight is its multi-threading capability.
 - The world first large-scale physics software fully multithreaded
- Geant4 version 10 series will be evolving.
 - Performance improvements (both in physics and computing)
 - Missing functionalities yet to be migrated to multithreading,
 - Additional APIs
 - Additional functionalities
 - New physics

| | G4MT prototype-9.4 (2011) | G4MT prototype-9 (2012) | 5 G4 10.0.beta (Jun.2013) G4 10.0 (Dec. 2013) | G4 10 series (2014~) |
|---|---|------------------------------------|--|-------------------------|
| • | Proof of principle Identify objects to be shared First testing | • MT code integrated into G4 | API re-design Example migration Further testing First optimizations Production ready Public release | • Further refinements |
| | | | Geant4 kernel update - M. Asai (SLAC) | |



ATLAS : "The 10% CPU improvement we gain from the move from G4 9.6 to 10.1 is invaluable to the collaboration."





- For three years we have provided support for running Geant4 on KNC.
 - ATLAS, CMS successfully multithreaded
- We will soon extend our support to KNL.
 - With KNL, thanks to x86 binary compatibility including the use of gcc, work-flow is tremendously simplified.

| System | Time to completion (5k events) |
|---|--|
| Xeon E5-2620 @ 2.1 GHz (12 cores, 24 threads) | 570 s |
| KNC (31s1P) @ 1.0 GHz (228 threads) | 1000 s |
| KNL (7210, quadrant mode, MCDRAM only) @ 1.3 GHz (255 threads) | 378 s (x3 improvement w.r.t. KNC) |
| KNL (shared library) | 480 s (25% slower than static library) |

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More memory-efficient, more HPC friendly

| Version | Intercept | Memory/thread |
|--------------|-----------|---------------|
| 9.6 (seq.) | 113 MB | (113 MB) |
| 10.0.p02-seq | 170 MB | (170 MB) |
| 10.0.p02-MT | 151 MB | 28 MB |
| 10.3.beta-MT | 148 MB | 9 MB |

Memory space required for Intel Xeon Phi 3120A Full-CMS geometry (GDML), 4 Tesla field, 50 GeV pi- (FTFP_BERT)

| # of CPU | # of threads | Speed-up factor | efficiency | |
|----------|--------------|--------------------|------------|------------------------------------|
| 10 | 80 | 79 | 98.8% | |
| 20 | 160 | 158 | 98.8% | |
| 40 | 320 | 317 | 99.0% | File Edit View Higtory Bookmarks I |
| 80 | 640 | 626 | 97.8% | (1) status.alcf.anl.gov/mira/acti |
| 160 | 1280 | 1251 | 97.7% | Argonne NATIONAL LABORATORY |
| 320 | 2560 | 2297 | 89.7% | |
| 640 | 5120 | 3555 | 69.4% | 1 - - |

Tachyon-2 supercomputer @ KISTI (South Korea) FTFP_BERT physics validation benchmark



Geant4 kern

- Geant4 has successfully run with a combination of MT and MPI on Mira Bluegene/Q Supercomputer (@ANL) with all of its 3 million threads
 - Full-CMS geometry & field
- I/O is the limiting factor to scale large concurrent threads:
 - Granular input data files, output data/histograms, etc.
 - 2017 work item
 - Targeting also Cori @ NERSC









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Sequential mode





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Multi-threaded mode



User's code migration

- If you have a running code with version 9.6 and you want to stick to sequential mode, you do not need to migrate. It should run with version 10.0.
 - Except for a few obsolete interfaces that you had already seen warning messages in v9.6.
- Migration of user's code to multi-threading mode of Geant4 version 10.0 should be fairly easy and straightforward.
 - Migration guide is available.
 - Geant4 users guides are updated with multi-threading features.
 - Most examples have been migrated to multi-threading.
 - Geant4 tutorials based on version 10.0 has already started.
- G4MTRunManager collects run objects from worker threads and "reduces".
- Toughest part of the migration is making user's code thread-safe.
 - It is always a good idea to clearly identify which class objects are thread-local.
- Every file I/O for local thread is a challenge
 - Input : primary events : examples are offered in the migration guide.
 - Output : event-by-event hits, trajectories, histograms



- G4TessellatedSolid
 - Generic solid defined by a number of facets (G4VFacet)
 - Facets can be triangular (G4TriangularFacet) or quadrangular (G4QuadrangularFacet)
 - Constructs especially important for conversion of complex geometrical shapes imported from CAD systems
 - But can also be explicitly defined:
 - By providing the vertices of the facets in *anti-clock wise* order, in *absolute* or *relative* reference frame
 - GDML binding
- G4ExtrudedSolid is re-implemented to internally use G4TessellatedSolid.





Geometry updates – New solid library

- An important effort was begun in the last few years to write a new solid library, reviewing at the algorithmic level most of the primitives and provides an enhanced, optimized and well-tested implementation to be shared among software packages.
- In most cases considerable performance improvement was achieved.
 - For example, the time required to compute intersections with the tessellated solid was dramatically reduced with the adoption of spatial partitioning for composing facets into a 3D grid of voxels.
- Such techniques allow speedup factors of a few thousand for relatively complex structures having of order 100k to millions of facets, which is typical for geometry descriptions imported from CAD drawings.
 - Consequently, it is now possible to use tessellated geometries for tuning the

precision in simulation by increasing the mesh resolution, something that was not possible before.



| Method | Speedup |
|--|---------------|
| Inside | 2423x |
| DistanceToIn | 1334x |
| DistanceToOut | 1976x |
| Information | Value |
| Number of facets | 164.149 |
| Number of voxels | 100.000 |
| Memory saved compared with original Geant4 | 22% (51MB) |

Boolean Solids

- Solids can be combined using boolean operations:
 - G4UnionSolid, G4SubtractionSolid, G4IntersectionSolid
 - Requires: 2 solids, 1 boolean operation, and an (optional) transformation for the 2nd solid
 - 2nd solid is positioned relative to the coordinate system of the 1st solid
 - Result of boolean operation becomes a solid. Thus the third solid can be combined to the resulting solid of first operation.
- Solids to be combined can be either CSG or other Boolean solids.





Geometry updates – New "multi-union" solid

G4MultiUnion* munion_solid = new G4MultiUnion("UnitedBoxes");

```
for( int i=0 ; I < nNode ; i++)
{
  G4Box* aBox = new G4Box(...);
  G4ThreeVector pos = G4ThreeVector(...);
  G4RotationMatrix rot = G4ThreeVector(...);
  G4Transform3D tr = G4Transform3D(rot, pos);
  munion_solid -> AddNode( *aBox, tr );
}
```

munion_solid -> Voxelize();



Note : G4MultiUnion is a solid. Use it to create a logical volume.



Geometry updates - New "multi-union" solid

- In addition to a full set of highly optimized primitives and a tessellated solid, the library includes a new "multi-union" structure implementing a composite set of many solids to be placed in 3D space.
- This differs from the simple technique based on Boolean unions, with the aim of providing excellent scalability on the number of constituent solids.
- The multi-union adopts a similar voxelization technique to partition 3D space, allowing dramatically improved speed and scalability over the original implementation based on Boolean unions.



- Multiple/single scattering
 - Introduction of optional displacement on geometrical boundary
 - New G4LowEWenzalVIModel for low-energy applications
- Gamma processes
 - Photo-effect and Compton cross-sections at low-energy integrated
- High-energy models
 - Improvements in gamma->muons, positron->hadrons and positron->muons
 - Synchrotron radiation for all particle types
- Atomic de-excitation
 - New alternative fluorescence dataset (Bearden)
- New radiolysis process for water and silicon
 - Physics stage followed by physicochemical and chemical stage
- Introduction of phonon transport with a new concept of crystal
- Channeling effect in straight and bent crystal
- Lots of code refinements along with MT





- FTFP_BERT is now the recommended physics list for most of high-energy use-cases
- Generation of Isomer (a.k.a. metastable nuclides)
 - by default lifetime > 1 nsec
- Neutron_HP is extended to Particle_HP to cover p, d, t, α
- Alternative low-energy neutron model with GND (Generalized Nuclear Data) format
- Liege intra-nuclear cascade model (INCLXX) extended up to 20 GeV
- FTF model extended to nucleus-nucleus and antinucleus-nucleus interactions
- Radioactive decay redesigned with rare decay channels
- New hadron stopping models based on Bertini
- Decommission of LHEP and CHIPS models





Hadronic Model Inventory



New biasing scheme

- Event biasing (a.k.a. variance reduction) scheme has been fully revised at version 10.
- It allows treating many biasing options in coherent manner.
- Such options include:
 - Physics process biasing : alters physics process
 - Cross-section biasing, forced interaction, forced passage, etc.
 - Biasing final products of an interaction, e.g. distribution
 - Non-physics biasing : alters the transportation of particle
 - Geometrical importance, splitting / Russian roulette, weight window, etc.
- Easily extensible to new (or user-defined) options
- Well-integrated with built-in scoring functionalities.
- New examples are available.



Five of 100 MeV neutrons on Pb/Scinti calorimeter. Left : analogue simulation Right : splitting with geometrical importance and probability control.

New features in analysis, GUI and visualization

- New built-in fully-multithreaded histogramming tool
 - 1-D and 2-D histograms and scatter plots, n-tuples
 - Data format compatible with ROOT, XML, AIDA, CSV
 - Extensible to other format
- GUI and visualization
 - New Qt driver with OpenGL
 - Viewer properties and picking panel, dock-able widgets
 - Multithread output filtering
 - More than 30% faster drawing on OpenGL
 - Magnetic field lines







| Scopus | | | <u>Search</u> Sour | S. Agostir Geant4 | elli (: a | et al. simulation | toolki | t |
|--|------------------|---|--|----------------------------|--------------------------------------|--|-----------------------|---------------------------------------|
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ScienceDirect

J. Allison et al. Recent developments in Geant4

NIM A, vol. 835, pp. 186-225, 2016

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Highlights Abstract

Keywords

- 1 The evolution
- 1. The evolution of G4
- 2. Multithreading
- 3. Kernel functionalities
- 4. Recent developments in physics mod...
- 4.4. Results
- 5. Toolkit extensions
- 6. Validation
- 7. Outlook for the next decade
- Acknowledgments
- References

Figures and tables

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment

Volume 835, 1 November 2016, Pages 186-225

Recent developments in GEANT4

J. Allison^{a, b}, K. Amako^{c, a}, J. Apostolakis^d, P. Arce^e, M. Asai^f, T. Aso^g, E. Bagli^h, A. Bagulyaⁱ, S. Banerjee^j, G. Barrand^k, B.R. Beck^l, A.G. Bogdanov^m, D. Brandtⁿ, J.M.C. Brown^o, H. Burkhardt^d, Ph. Canal^j,

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https://doi.org/10.1016/j.nima.2016.06.125

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Highlights

- Multithreading resulted in a smaller memory footprint and nearly linear speed-up.
- Scoring options, faster geometry primitives, more versatile visualization were added.
- Improved electromagnetic and hadronic models and cross sections were developed.

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New areas of User Applications

To provide you some ideas how Geant4 would be utilized...

Geant4 Applications in NASA Space Missions - M. Asai (SLAC)

Simulation of Radiation Events

- 63-MeV proton incident on a SiGe Heterojunction Bipolar Transistor (HBT)
- Iso-charge surfaces following a nuclear reaction

Courtesy of R.Reed (Vanderbilt U.) Geant4 kernel update - M. Asai (SLAC) SLAC

Observed and Predicted SEU Rate for an SRAM

- SRAM used on NASA Messenger spacecraft
- Observed Average SEU Rate:
 - 1x10⁻⁹ Events/Bit/Day
- Vendor predicted rate using CREME96:
 - 2x10⁻¹² Events/Bit/Day
 - Classical Method nearly a factor 500 lower than observed rate
- MRED rate (includes reaction products):
 - Between 1.3x10⁻¹⁰ and 1.3x10⁻⁹
 Errors/Bit/Day

Courtesy of R.Reed (Vanderbilt U.)

Comparison with Geant4

Simulation results agrees with experimental data within a factor of two in terms of the line intensities

Condensed Matter Physics in Geant4

•Phonon propagation, including focusing based on elasticity tensor (right)

•e-/h+ transport, including conduction band anisotropy and Luke-Neganov emission, under development (below)

e-/h propagation with Luke phonon emission in Ge crystal

Geant4 ke

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Bent crystal as a collimator

- Bent crystal can be used as a collimator to deflect particles of beam halo.
- This study will be extended for T-513 experiment at SLAC LCLS ESTB

SLAC

LSST (Large Synoptic Survey Telescope)

"Geant4 Applications for Modeling Molecular Transport in Complex Vacuum Geometries." J.Singal, J. Langton, R. Schindler, Int J Mod Sim Sci Comp, in press (arXiv:1302.2963)

symmetry

particle physics

Those exterior walls, made of concrete 10 feet thick, offer their own challenge. Based on computer simulations run with the particle physics software GEANT4, the walls are expected to reduce the resolution to about 30 centimeters.

In addition, the team must also prepare for the high radiation levels present just outside of the reactor units.

> ors (shown here in green) on either side of record the path of muons (represented by the nrough the reactor. By determining how the ectors, scientists will compile the first picture of

with Shawna X.

As time ticks down to the restart of the Large Hadron Collider, scientists are making sure their detectors run like clockwork.

age

SLAC

Journal of Environmental Radioactivity

Volumes 162–163, October 2016, Pages 118–128

Evaluating remediation of radionuclide contaminated forest near Iwaki, Japan, using radiometric methods

D.C.W. Sanderson^{a, L}, Matsuzaki^d, A.J. Cresswell^a, K. Tamura^b, T. Iwasaka^c, K. Matsuzaki^d

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Received 24 December 2015, Revised 10 May 2016, Accepted 15 May 2016, Available online 24 May 2016

Muon tomography for nuclear threat detection

Muon tomography for nuclear threat detection

Article | OPEN

Uncovering Special Nuclear Materials by Low-energy Nuclear Read

P. B. Rose, A. S. Erickson 🏁, M. Mayer, J. Nattress & I. Jovano

Scientific Reports 6, Article number: 24388 (2016) doi:10.1038/srep24388 Download Citation Applied physics Imaging techniques Figure 1: Illustration of the imaging method using a low-energy nuclear reaction radiation source.

Ongoing developments in kernel

to be delivered in 10.5 or within a couple of years

C++11 threading

- All POSIX threading implementation updated to C++11 threading
 - Windows + MT enabled
- Windows + MT + shared libraries requires "construct-on-first-use" paradigm
 - If you are not using Windows+MT+SL, you don't need to change your code.

header extern G4PART DLL G4Allocator<G4PrimaryParticle>* aPrimaryParticleAllocator; inline void* G4PrimaryParticle::operator new(size t) ł if (!aPrimaryParticleAllocator) aPrimaryParticleAllocator = new G4Allocator<G4PrimaryParticle>; old return (void*) aPrimaryParticleAllocator->MallocSingle(); } source G4ThreadLocal G4Allocator<G4PrimaryParticle>* aPrimaryParticleAllocator = 0; header extern G4PART DLL G4Allocator<G4PrimaryParticle>*& aPrimaryParticleAllocator(); New in v10.5 inline void* G4PrimaryParticle::operator new(size t) { return (void*) aPrimaryParticleAllocator()->MallocSingle(); new } source G4Allocator<G4PrimaryParticle>*& aPrimaryParticleAllocator() G4ThreadLocalStatic G4Allocator<G4PrimaryParticle>* instance = new G4Allocator<G4PrimaryParticle>(); return instance; }

C++11 threading

- G4THitsVector
 - Similar to G4THitsMap but smaller memory footprint
- G4StatAnalysis
 - Low memory footprint class for basic statistics
 - Size: 2 int, 2 doubles (constant) Compatible with G4THitsMap and G4THitsVector
 - It offers:
 - Mean
 - Standard deviation / variance
 - Relative error
 - FOM
 - Efficiency
 - May replace G4StatDouble

New in v10.5

Sub-event parallelism

- Geant4 MT was initially designed to process events in parallel.
 - Each event is tasked a thread.
 - Independence of threads makes perfect scaling of throughput with #threads
 - But scheme assumes events are small enough to fit into the memory of one thread
- Sub-event parallelism generalizes this approach:
 - To serve the case of applications requesting large memory per event:
 - e.g. ALICE, HL-LHC, air shower
 - One event is split into "sub-events"
 - e.g. each few primary tracks = a sub-event
 - Split method is obviously user-dependent.
 - Each sub-event is sent to a thread, and merged back to the original full event later
 - Geant4 will provide tools to easily enable this feature
 - All the current API's should be preserved.

Sub-event parallelism

- Constraint all the current API's must be preserved.
 - Special G4UserPrimaryGeneratorAction class will be introduced, and will be used only in the master thread.
 - It has SplitEvent() and MergeEvent() methods.
- Constraint Objects instantiated by a worker thread must be deleted by the same worker thread.
 - Only the objects of G4PrimaryVertex and G4PrimaryParticle will be instantiated in the master thread and associated to a G4Event object, and G4Event (sub-event) is tasked to a thread.
 - After the merger, Hit and trajectory objects created by a worker thread will be sent back to the corresponding worker thread for deletion.
- Time scale of the development :
 - Source code : to be finished by May 2019
 - An example : to be finished by September 2019

Unified tracking mechanism for exotic particles

- Each elementary particle and light ion (up to alpha) in Geant4 is represented by a dedicated G4ParticleDefinition class object, and each G4ParticleDefinition class object has its own G4ProcessManager class object to register processes for that particle.
 - ~100 G4ParticleDefinition objects
- This is not the case for ions. Though G4ParticleDefinition class object is created for each ion (A, Z, E, J), they all share one G4ProcessManager class object to register processes for all ions, assigned to G4GenericIon artificial class.
 - ~7000 G4ParticleDefinition objects
- G4MuonicAtom was introduced. Theoretically, any ion may become a muonic atom. Though G4ParticleDefinition class object is created for each muonic atom (A, Z, E, J), they all share one G4ProcessManager class object to register processes for all muonic atoms.
 - G4ProcessManager for muonic atom is different from one for ions.
 - Mechanism of sharing G4ProcessManager was duplicated.
- In G4DNA, radicals (e.g. OH⁻) are treated in the same manner. Hyper-nucleus physics is in the scope.
 - ~20000 G4ParticleDefinition objects in four different categories

Unified tracking mechanism for exotic particles

- Uniform, transparent and extendable treatment is required.
 - Likely particles of no more than two categories co-exist. Performance overhead must be avoided and at the same time clean code structure is desirable.
- G4SteppingManager is already cleaned up. There is no longer #ifdef, there is no longer indirect access to G4PrcessManager via G4GenericIon (or G4GenericMuonicAtom, etc.).
 - G4IonTable is updated to ensure this.
- Remaining work Split G4IonTable class
 - G4IonTable::GetMuonicAtom() will be moved to new G4MuonicAtomTable.
 - Hyper-nucleon, radicals, will have their own "table" class.
 - Clean way to enable extendibility for yet another particle family without overhead
 - Plan to finish in the coming year.

Revisit / retreat production thresholds and physics process framework

• Production thresholds ("cuts") initially considered as an issue fundamental enough to be taken care at the kernel class level.

| Particle produced | Production process | Motivation |
|----------------------|-----------------------|--|
| eî— | Ionization | Heavy production (limited by energy binding to atoms). These are actually "recoil electrons". Threshold needed to limit the production. |
| eî+ | Conversion | No divergence nor heavy production. Use case : production cut in mountain rock for, e.g., dark matter experiments. |
| γ | Bremsstrahlung | Cross-section divergence (actually limited by dielectric effects at very low energies). Threshold needed to limit the production. |
| p (ions) | Hadron elastic | Threshold on recoil proton, e.g. n scattering on proton, ejecting it. Mechanism adapted for ions. Threshold defines the "visibility" cut. |

• Study has started.

Refactoring transportation

- The "transportation" is a Geant4 process
- It manages the navigation in the geometry:
 - It cares about volume boundaries
 - It takes into account the fields in the propagation of particles sensitive to such fields
- Currently, only one transportation object exists in the memory:
 - Either G4Transportation,
 G4CoupledTransportation or
 G4ITTransportation
 - It deals with all particle types:
 - neutral and charged particles, optical photons, phonons, etc.
 - Results in frequent "if" branches
 - on the charge to decide to apply field computation or not,
 - to use group velocity or not

Sources of CPU consumption Geant4 CMS simulation Courtesy of Vladimir Ivanchenko

Refactoring transportation

- Idea is to provide at least two flavors of transportation that co-exist:
 - One for charged particles, one for neutral particles
 - On-the-fly switching of steppers could also be considered.
 - Eventually one also for optical photons
 - As velocity calculations differ from other particles
- Case of other fields -e.g. gravitation- could be treated with more transportation flavors
- Further extensions/specializations to be also considered:
 - VecGeom navigation: optimized/vectorized, implementation with modern C++
 - À la DagMC: direct and efficient navigation in CAD geometries
 - DNA navigation: better serve the case of radicals
- Revision extended to "Coupled Transportation":
 - Transportation process dealing with several parallel geometries simultaneously
 - Has many use-cases: e.g. layered-mass geometry: allows to switch between several representation of a same detector, depending on particle
- Study in progress. Plan to deliver first implementations in 2019 as an option in G4VModularPhysicsList::AddTransportation().

Geant4 – the Future

- Physics of O(100TeV)
- Neutrino interactions
 - Should come with enriched event biasing options
- Electron/hole drift in semiconductor
- More phonon physics
- Channeling effects and physics with crystal structure in general
 - X-ray diffraction
- Single atom irradiation
- Target material polarization
- Chemical reactions of radicals in DNA-scale
- New domains ?
- Note : Geant4 kernel is robust enough over 20 years of evolution. This stability enables risk-free extensions to new physics.

New computing trends

- HPC and cloud friendliness
 - Seamlessly combining MPI and MT
 - Smart data collection from millions of threads
- Code re-engineering
 - Solid library, EM physics
 - Splitting transportation process
- GPU as a co-processor
 - Off-loading some calculations to GPU, e.g. EM physics, thermal neutron physics, DNA physics and chemical processes, etc.
- Will be integrated into Geant4 with (hopefully) minimum API changes

To sum up

- Geant4 is a general purpose Monte Carlo simulation tool for elementary particles passing through and interacting with matter. It finds quite a wide variety of user domains including high energy and nuclear physics, space engineering, medical applications, material science, radiation protection and security.
- 2018 is the 20th year anniversary of public release of Geant4. After 20 years with several architectural evolutions, Geant4 is still steadily evolving.
 - Latest evolution was Geant4 version 10.0 released in December 2013 that is the first fully multithreaded general-purpose large-scale physics software in the world.
 - New physics models for coming experiments, e.g. hadronic model for multi-TeV regime (for energy frontier), specialized EM model for noble liquid (e.g. liq.Xe) and neutrino physics model (for intensity frontier)
- Given Geant4 is nowadays mission-critical for many users including all HEP experiments, space missions, medical applications, etc., Geant4 is to be kept maintained and still evolving for at least next decade.

