Full Simulation of HEP Detectors with Geant4

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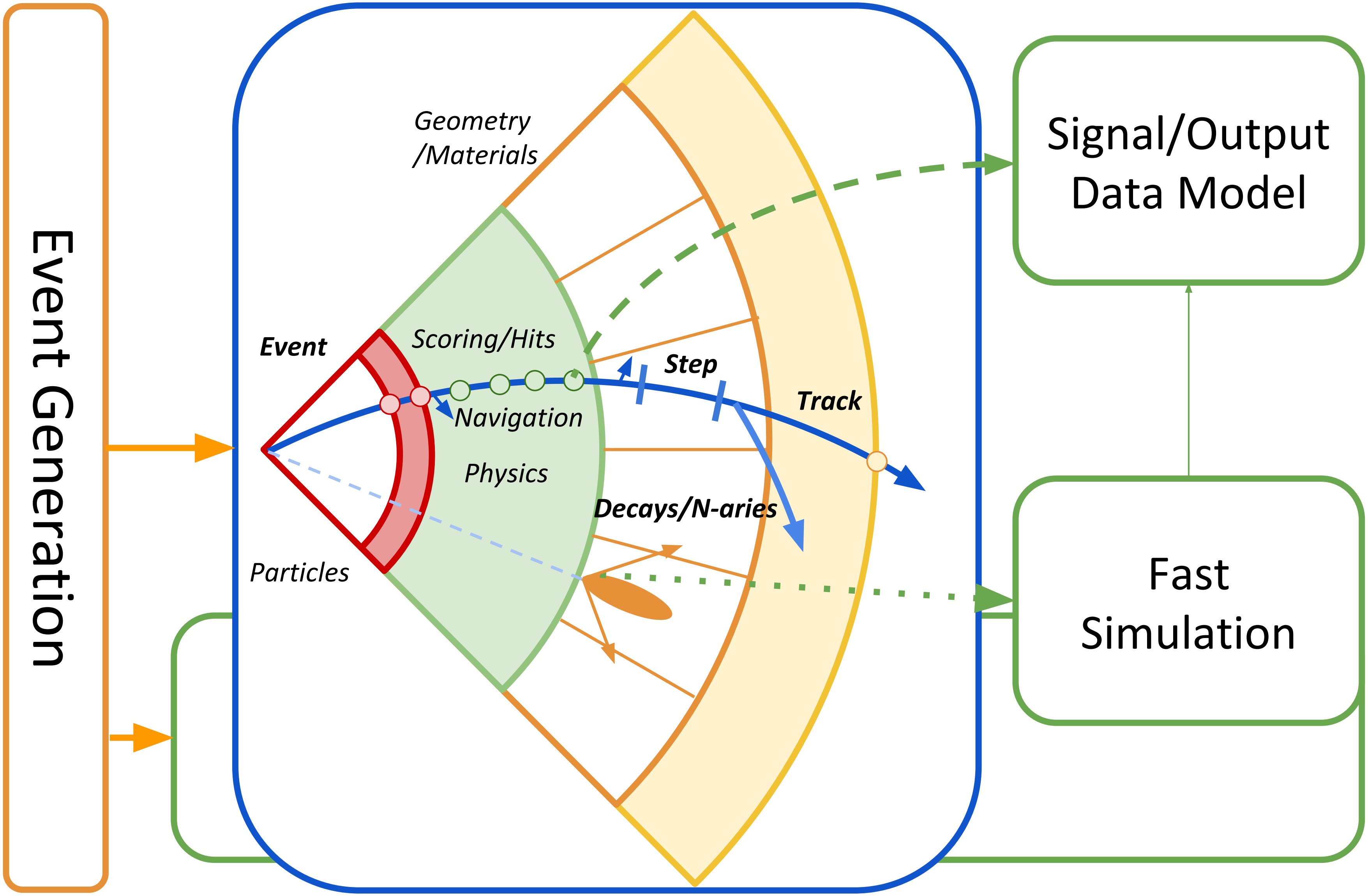
Workshop on Efficient Computing for HEP
Edinburgh 17-18 February 2020



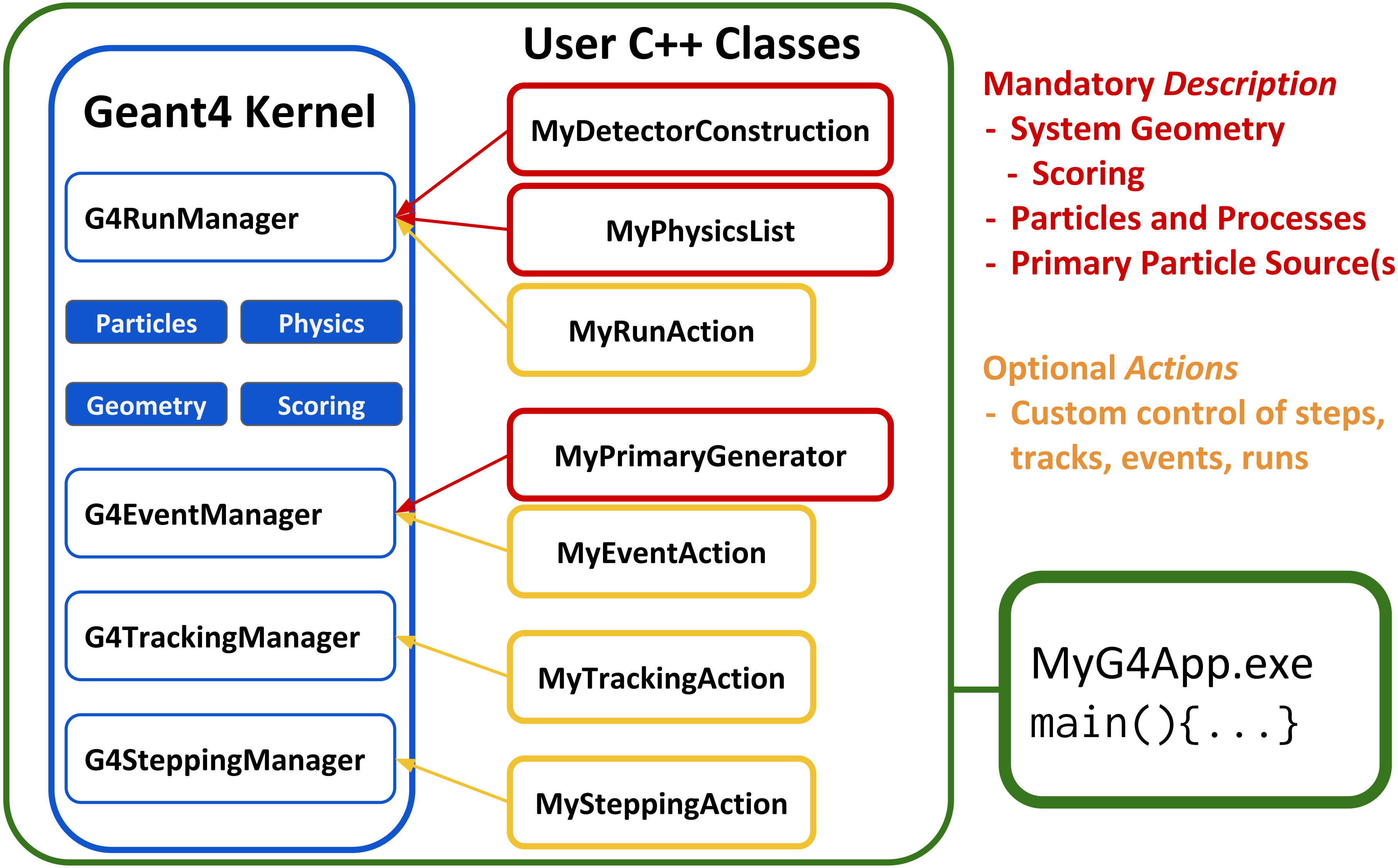
Scope of Full Detector Simulation

Event generators and Fast Simulation in other talks

Software for Detector Simulation

- **Primary** software used by HEP is **Geant4(*)**
  - *Others like Fluka, MCNPX, EGSnrc, used in limited or very specialized applications*

- (*) "*Geant4*" **not** "Geant", "4" **isn't** a version, and "Geant4" is **not an acronym**...

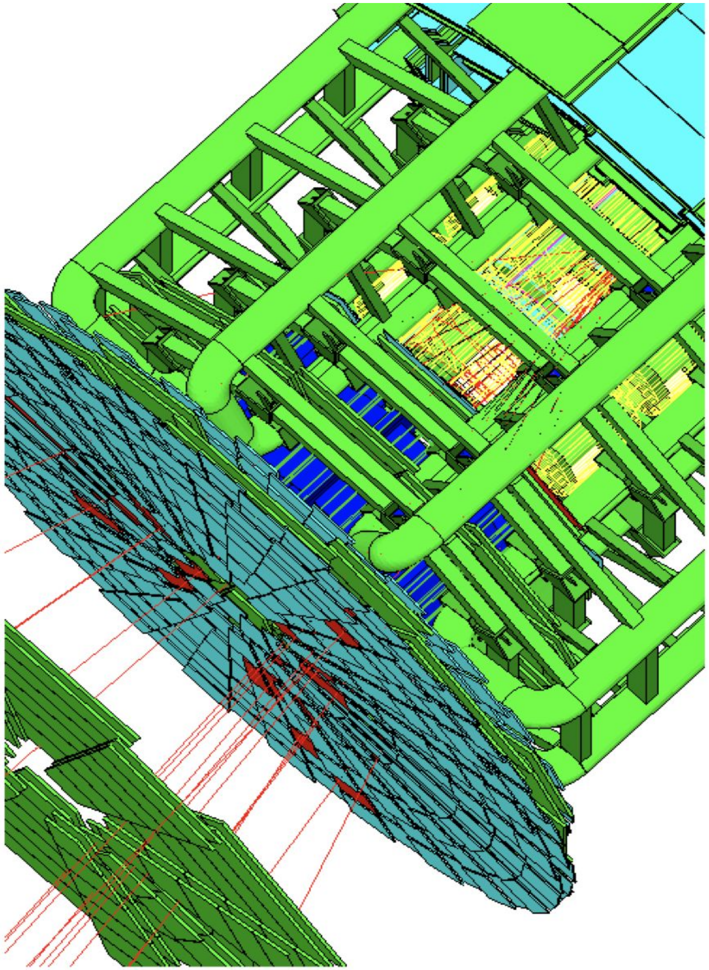


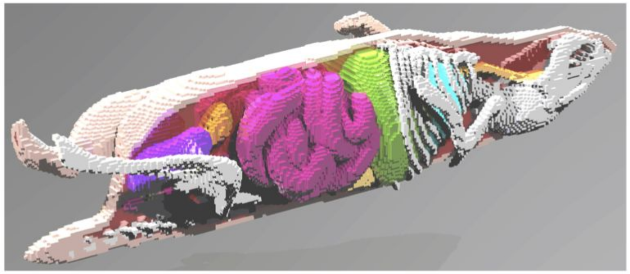
Geant4 in Brief

A general purpose **C++ Monte Carlo simulation toolkit** for elementary particles passing through and interacting with matter

Geant4 Capabilities: Geometry

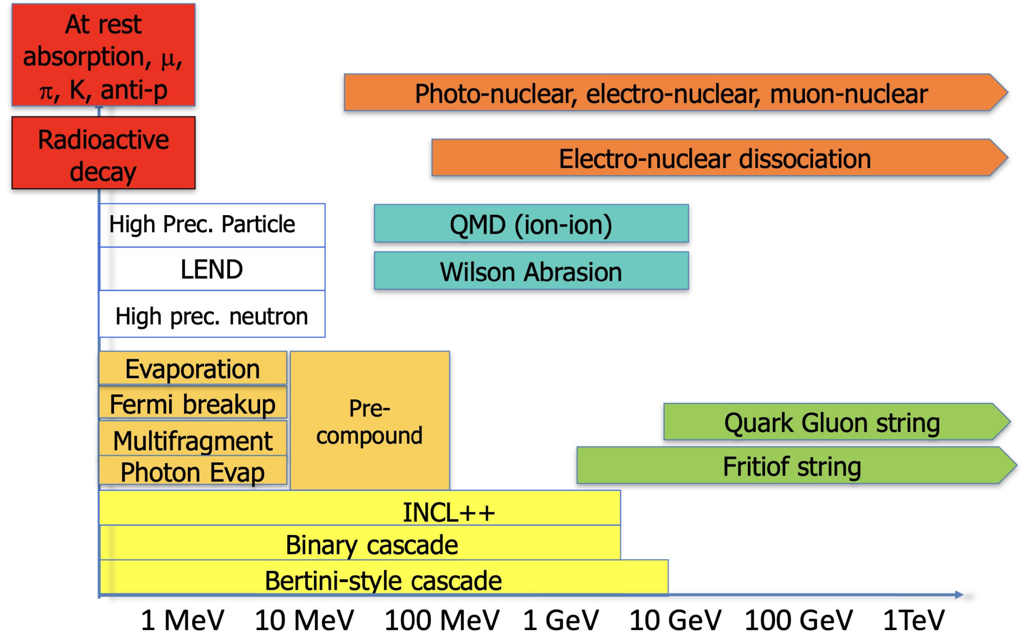
- Rich collection of shapes
  - *CSG, Union, Tesselated, User…*
- Arrange in a hierarchical or flat structure
  - *Handles up to O(10^9) volumes*
  - *Tools for creating and checking complex structure*
  - *Third party tools for CAD import*
- Fast navigation in complex models via automatic voxelization
- Optional use of **VecGeom** for improved performance with some shapes

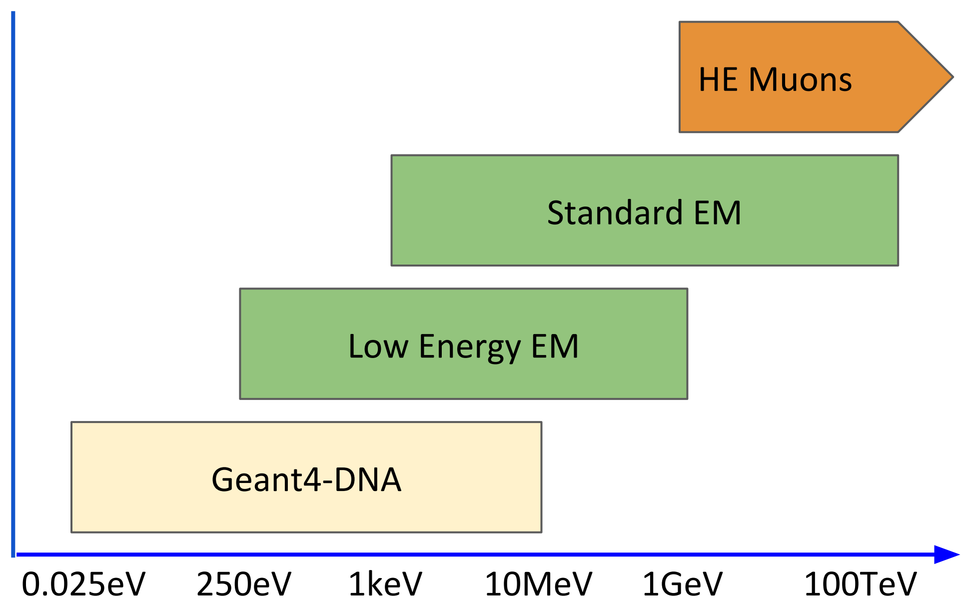




Geant4 Capabilities: Physics Models

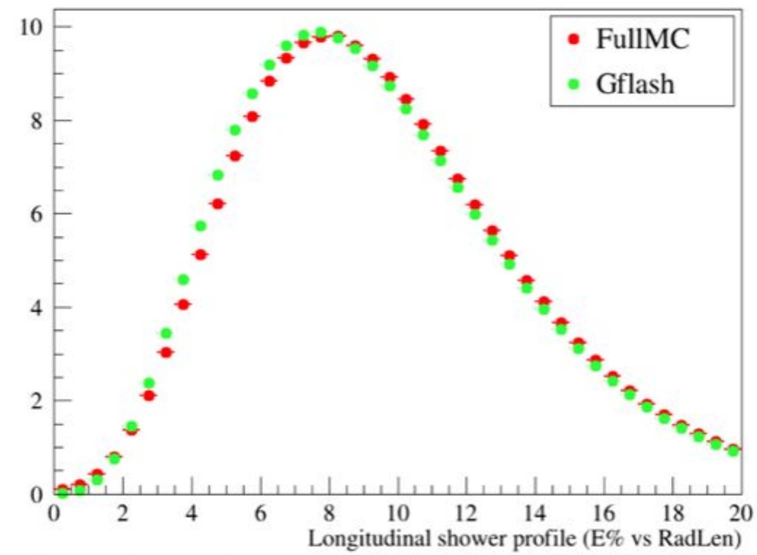
- Rich range offered:
  - *Electromagnetic*
  - *Hadronic/Nuclear*
  - *Photon/lepton-hadron*
  - *Optical photons*
  - *Decays*
  - *Shower parametrization*
  - *Event biasing*
  - *User defined*
- Cover energy ranges from sub eV to multi-TeV
- Alternative models to allow user to optimize for their application,
  - *e.g. trade speed for accuracy*

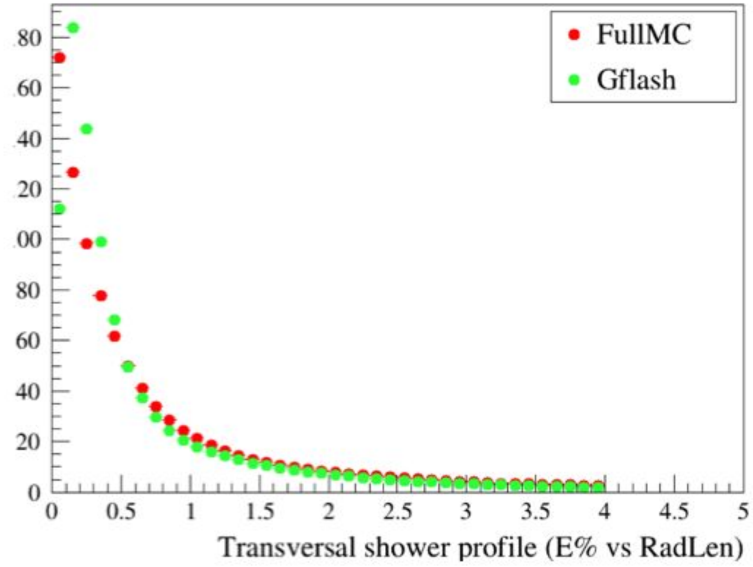


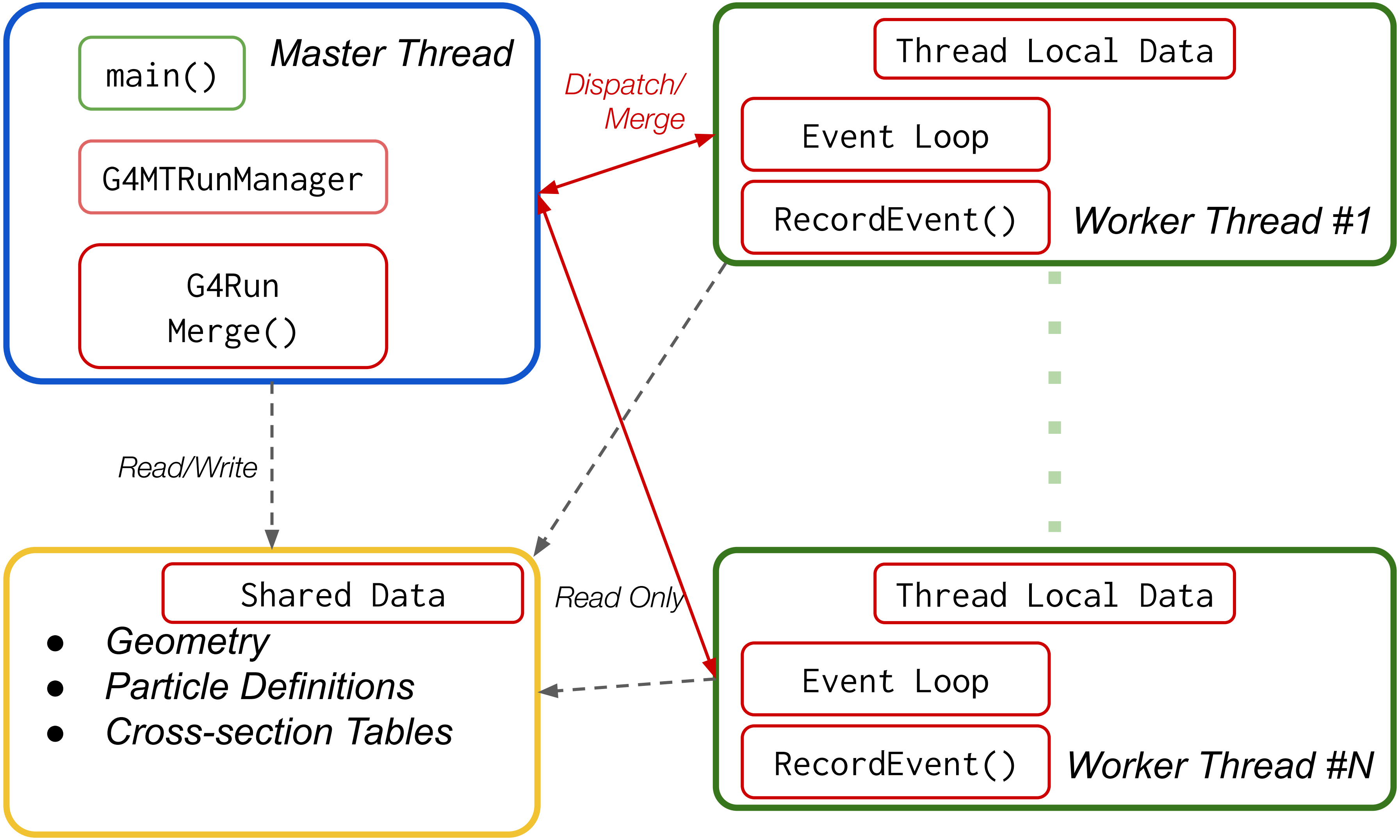


Geant4 Capabilities: Fast Methods

- **Fast simulation** hooks to override detailed tracking:
  - *In defined geometric regions...*
  - *… for given particle types...*
  - *… with a specified model*
- **Parallel world** geometry
  - *E.g. average density bulk for low energy EM particles in shower, full geometry for muons*
- Wide range of **biasing** methods/hooks provided
  - *Importance sampling*
  - *Primary/leading particle*
  - *Adjoint/Reverse Monte Carlo*
  - *Generic/extensible physics-based*
  - *Generic/extensible add/remove, e.g. splitting, Russian roulette*

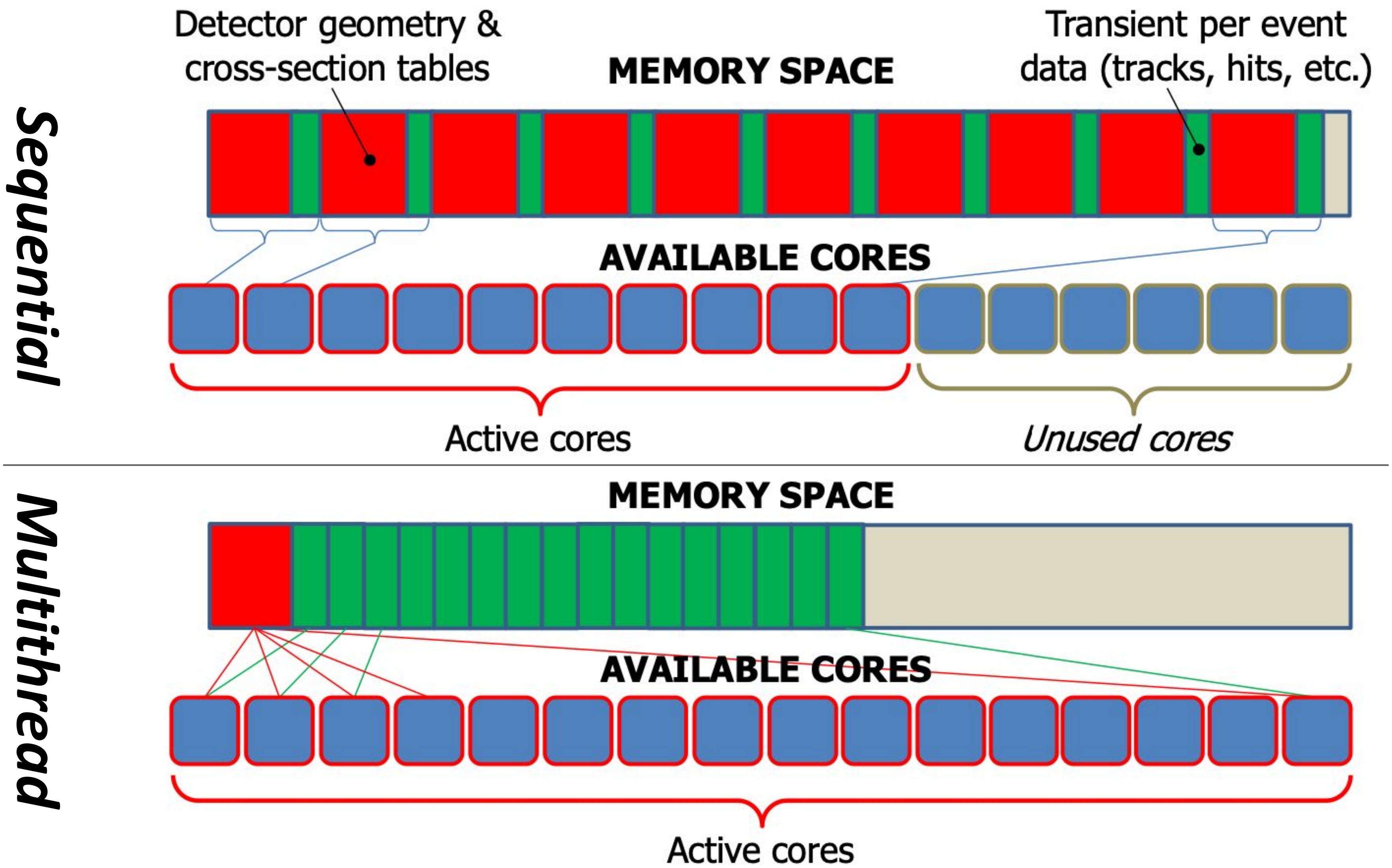






Geant4 Capabilities: Multithreading

Event level parallelism
Minimal API changes for Sequential->MT user code



Multithreading: Efficient Resource Usage

Multithreading yields better usage of Cores+Memory

Geant4 Development History

R&D Phase (RD44)

- Early discussions, e.g. CHEP 94
- Dec 1994: CERN/RD44 starts
- Apr 1997: Alpha release
- Jul 1998: Beta release
- **Dec 1998: Geant4 1.0**

Production Phase

- Several major architectural changes
  - STL migration, cuts-per-region, parallel worlds...
- **Multithreading**: Developed 2011-2013 (G4MT 9.4-9.6)
- **Dec 2013: Geant4 10.0.0 public release with Multithreading**
  - ***With minimal changes to user code!***
- **Dec 2019: Geant4 10.6.0**

Scopus

As of 02/2020

Search Sources Lists SciVal

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12,644 documents have cited:

GEANT4 - A simulation toolkit

Agostinelli S., Allison J., Amako K., Apostolakis J., Araujo H., Arce P., Asai M., (...), Zschiesche D.

(2003) Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 506 (3) , pp. 250-303.

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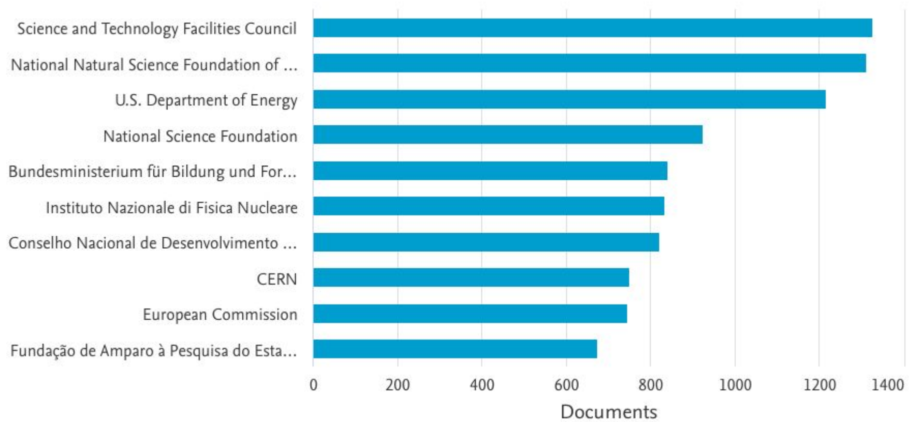
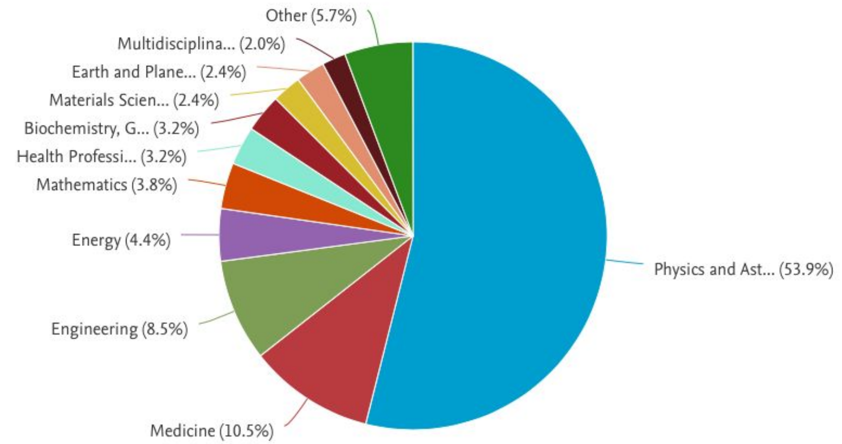
Documents by subject area

Documents by funding sponsor

Compare the document counts for up to 15 funding sponsors.





Geant4 - A simulation toolkit

[NIM A, vol 506(3), pp250-303, 2003]

Significant use across **many** research areas, **considered mission critical for HEP**

As of 02/2020

Scopus Search Sources Lists SciVal Create account

647 documents have cited:

Recent developments in GEANT4

Allison J., Amako K., Apostolakis J., Arce P., Asai M., Aso T., Bagli E., (...), Yoshida H.

(2016) Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 835 , pp. 186-225.

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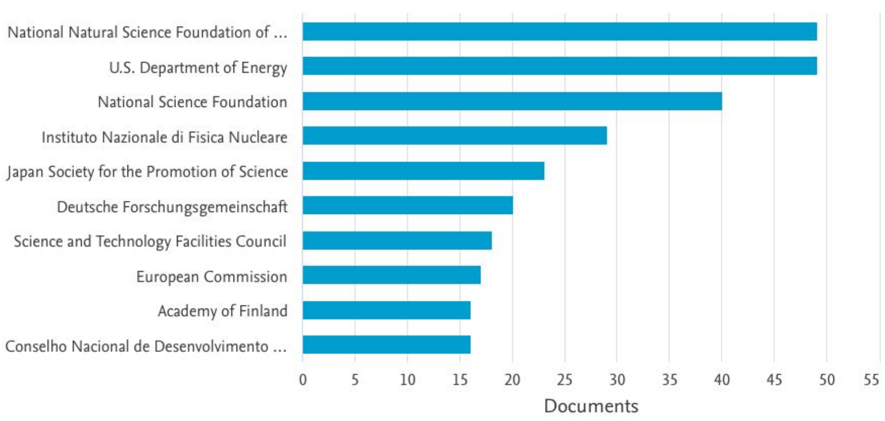
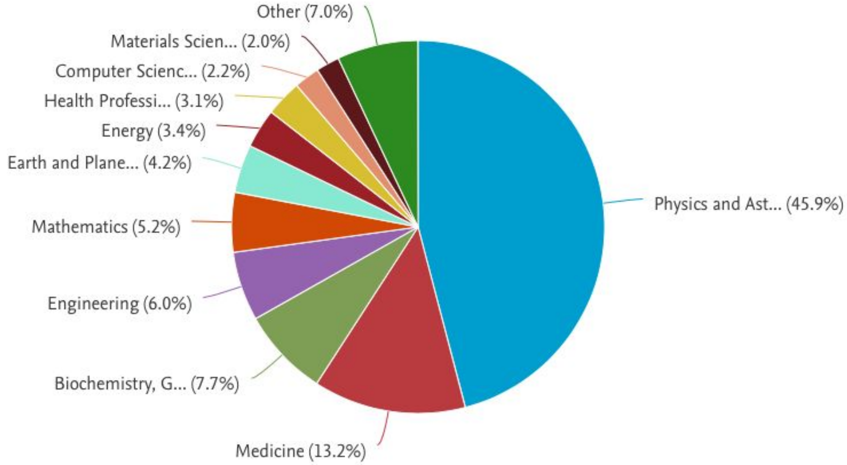




Recent developments in Geant4

NIM A, vol 835, pp 186-225

Reflects major upgrades to **capability** and **usability** of version 10 series

Collaborator Login

GEANT4
A SIMULATION TOOLKIT

Download | User Forum
Contact Us | Bug Reports

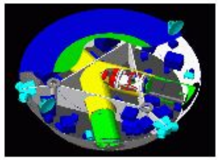
Overview

Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science. The three main reference papers for Geant4 are published in Nuclear Instruments and Methods in Physics Research A 506 (2003) 250-303, IEEE Transactions on Nuclear Science 53 No. 1 (2006) 270-278 and Nuclear Instruments and Methods in Physics Research A 835 (2016) 186-225.

Applications

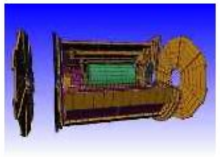
A sampling of applications, technology transfer and other uses of Geant4

User Support



Getting started, guides and information for users and developers

Publications



Validation of Geant4, results from experiments and publications

Collaboration

Who we are: collaborating institutions, members, organization and legal information

printer-friendly version

News

- *6 Dec 2019*
  Release 10.6 is available from the download area.
- *17 Apr 2019*
  Patch-01 to **release 10.5** is available from the source archive area.

Events

- Geant4 Course at the 17th Seminar on Software for Nuclear, Sub-nuclear and Applied Physics, Porto Conte, Alghero (Italy), **24-29 May 2020**.
- 25th Geant4 Collaboration Meeting, IRISA Laboratory, Rennes (France), **21-25 September 2020**.
- 4th Geant4 International User Conference at the Physics-Medicine-Biology Frontier, Napoli (Italy), **19-21 October 2020**.

Past Events

Geant4 Collaboration

~130 members, ~30FTE

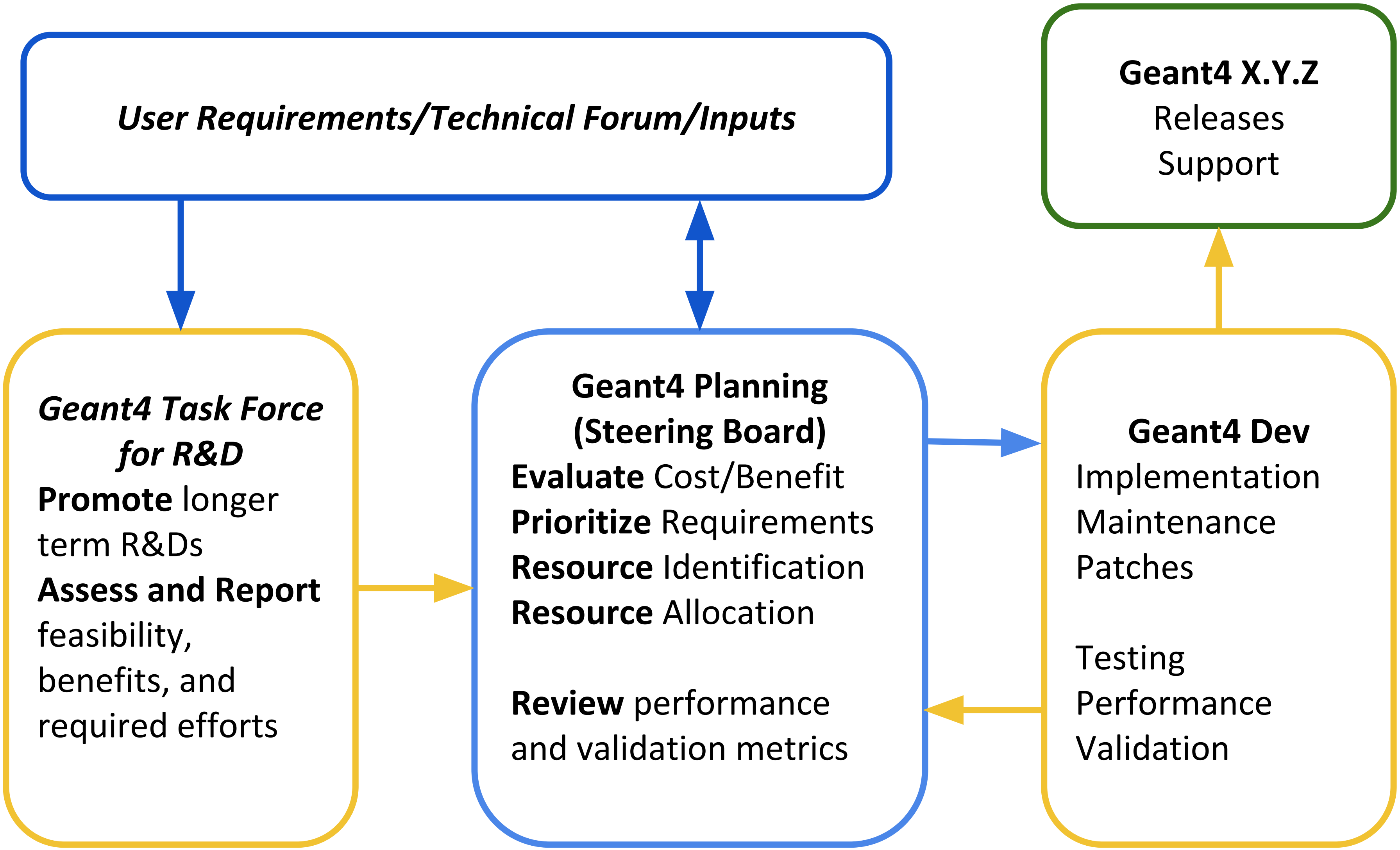
2 UK members from HEP, 4 from medicine, industry

Geant4 Development Principles

1. Provide excellent **support** to users
2. **Maintain** the toolkit for long-term **sustainability**
   a. *Flexible and easy **integration** with user/project codes*
3. Improve the **precision and energy range of physics models**
4. Improve the **performance** of the toolkit

*Recognizes **mission critical** nature of Geant4 for HEP*

*First three principles are **crucial** to realize the fourth*

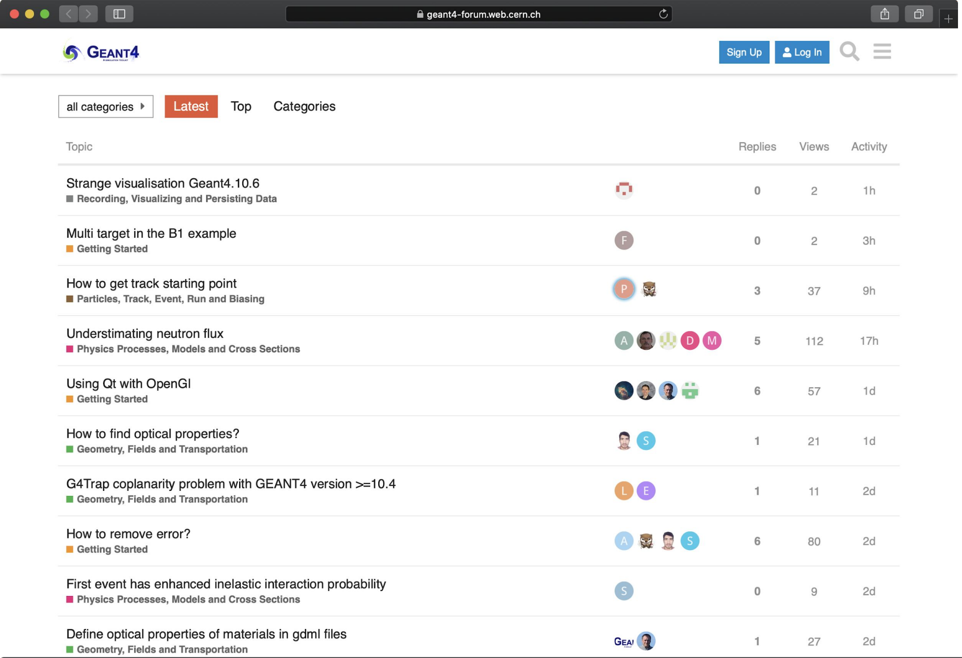


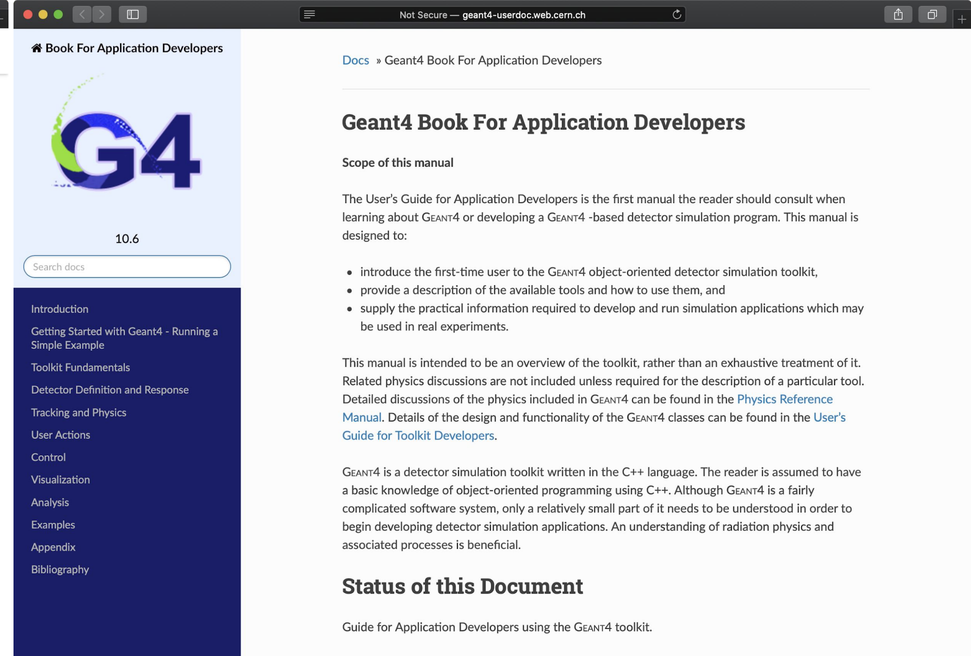
Geant4 Development Process

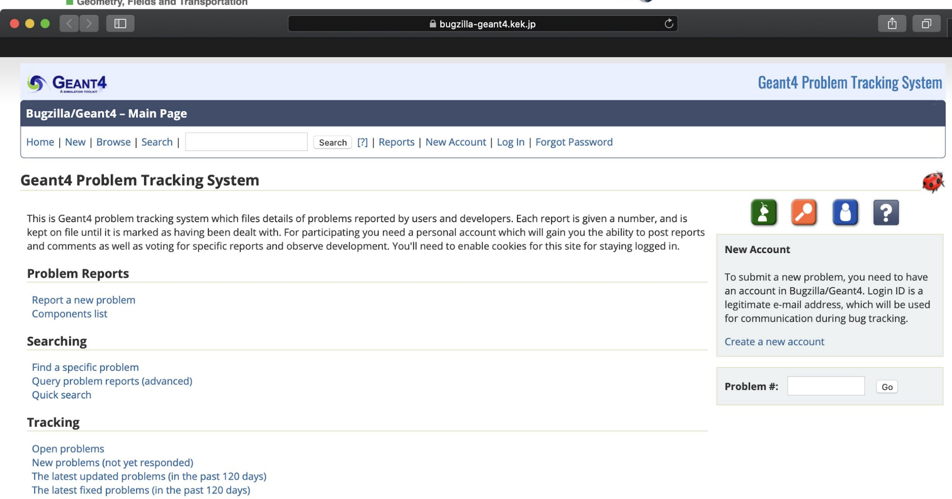
Provides balance between the four principles

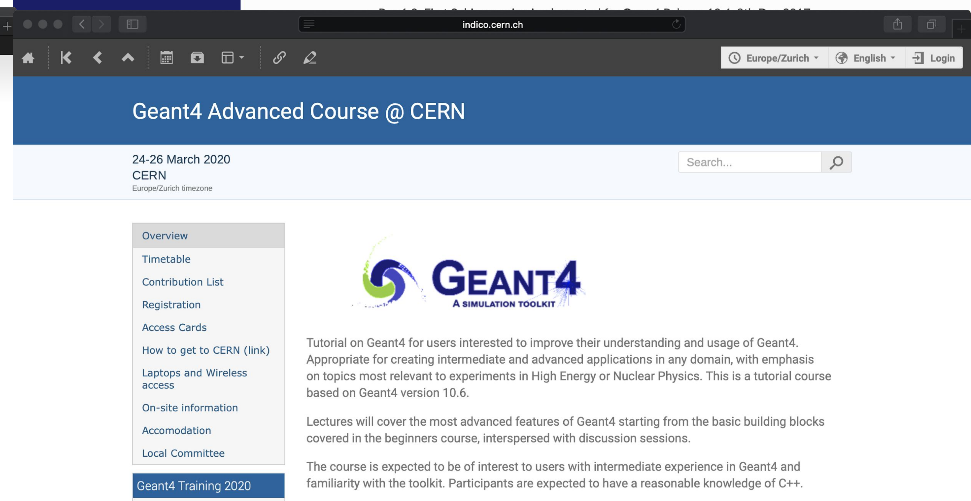
Geant4 Task Force for R&D

- Promote and survey research activities:
  - *Potential **software architect** updates to Geant4*
  - *use of **emerging technologies/computing architectures** of benefit to Geant4*
- Ensure the visibility of such explorations and act as the focal point for such **activities inside and outside of the Collaboration**
- Where appropriate, conduct benchmarking comparison and provide/assist communication/support among R&D activities
- Make timely assessment reports to Steering Board with **solid proof of benefits**
- ***Based on assessments of this Task Force, once a concrete and beneficial architectural revision is identified, the Steering Board launches a new, dedicated, task force to create workflow, estimate required resources and drive that particular development for integration into the code base.***
  - ***As was done for Multithreading and prior revisions***



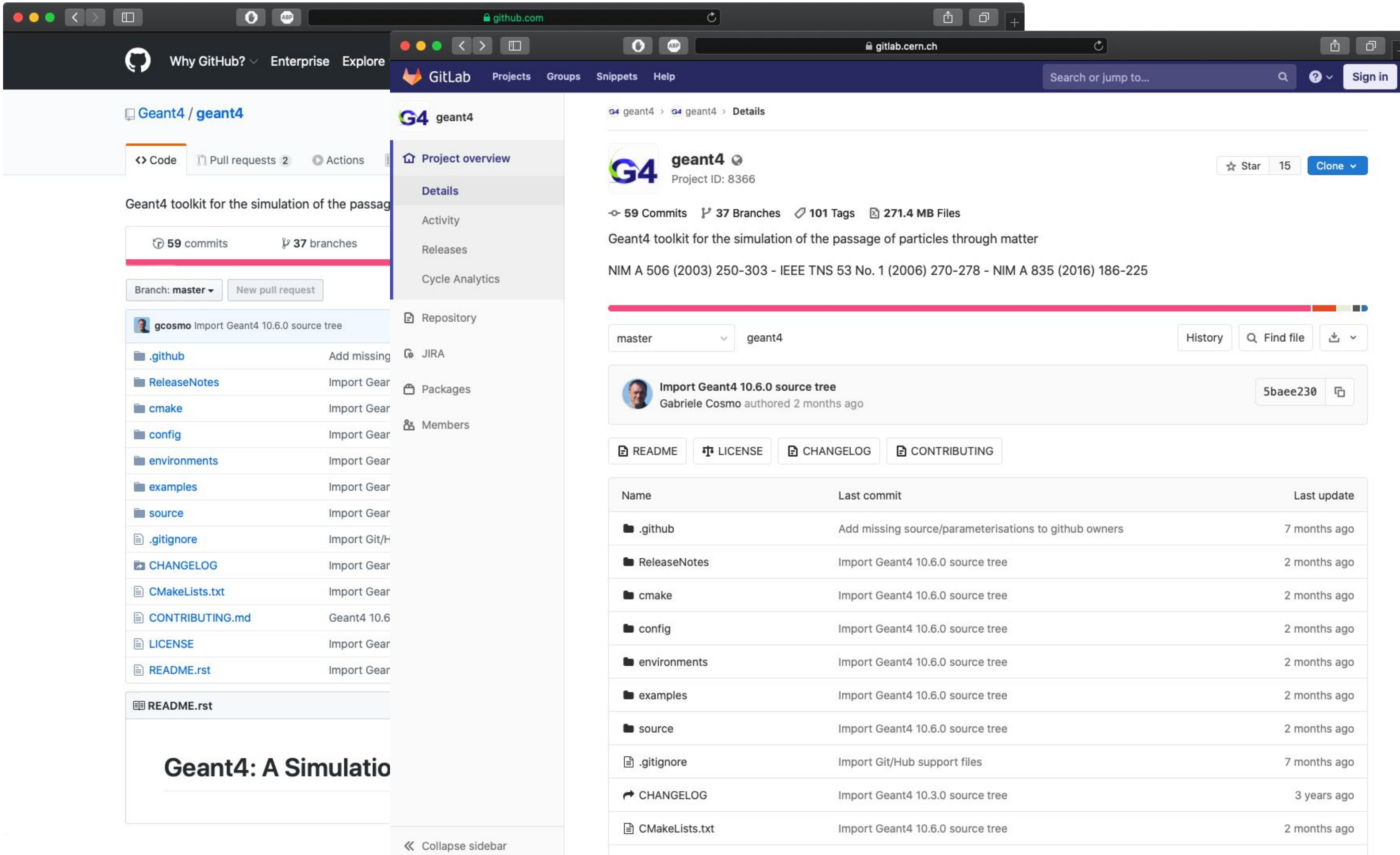






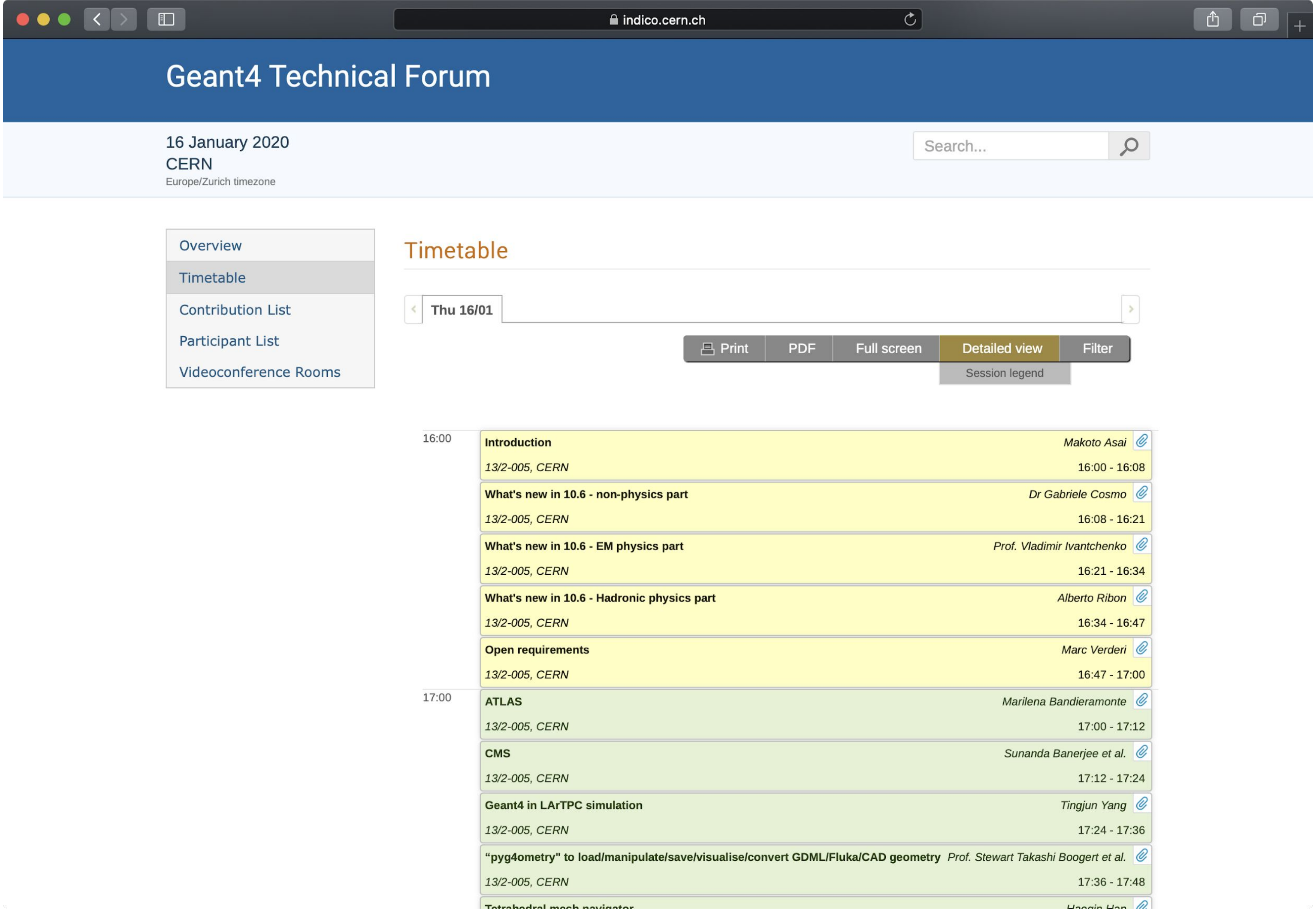
Support and Sustainability

A critical foundation for performance: best practice, early problem reporting



GitLab/Hub

Releases/Patches/Betas



Technical Forum

Regular meetings to collect user requirements to guide **workplan and priorities**, and update the community on new developments

HEP Requirements (LHC, CALICE, FCC)

- Only a flavour!
  - *Hadronic models for c and b-mesons*
  - *"Sub-event" parallelism to handle high-memory events*
  - *Very high energy physics effects (FCC-hh)*
  - *Navigation with VecGeom*
  - *Gamma polarization in high energy EM models*
- Plus bug reports and general support

Neutrino/Low Background Requirements

- Again, only a selection
  - *Specialized physics models for Liquid Argon detectors*
  - *Detailed output from hadronic cascades*
  - *Better performance for optical photons*
  - *Built-in neutrino interactions*
  - *Neutron self-shielding*
  - *Gamma induced neutron backgrounds*
- Plus bug reports and general support
  - *Particularly valuable for data-driven decays/cross-sections*

Continuous Testing

On each new GitLab Merge Request:

- *Code review by developers, quality checks (clang tools)*
- *Each change compiled and simple unit tests/applications run, ~45mins per change*

Nightly Testing

Set of pre-approved MRs: Unit/FPE/BoundsChecking tests, Valgrind, low statistics benchmarking and validation

- *~500 CPU hours per night on shared CERN-SFT resources*

Monthly/Release Candidate/Release Tests

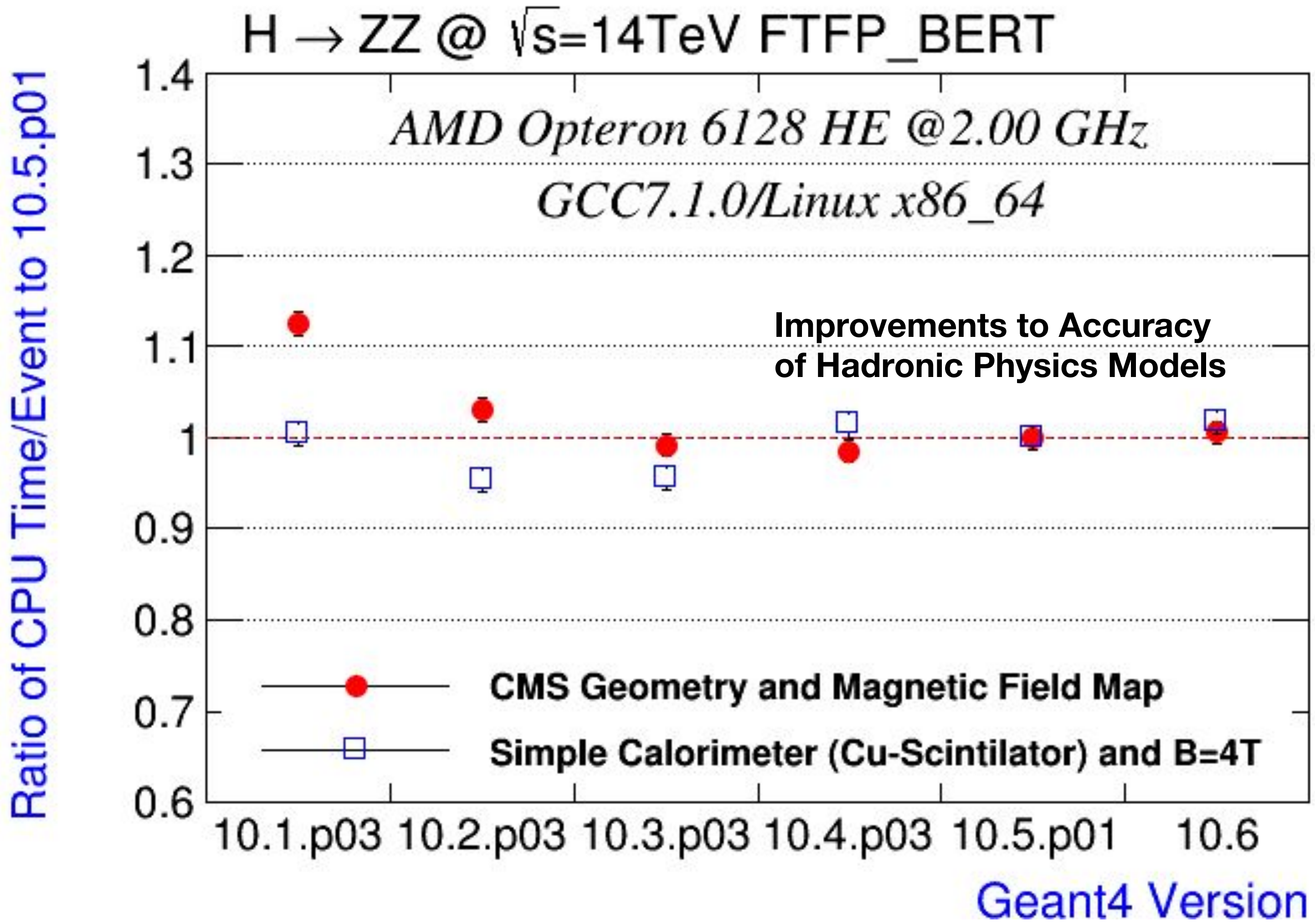
Detailed static analysis with Coverity

*High statistics **benchmarking** (OpenSpeedShop, IgProf) and **validation** on FNAL Wilson Cluster*

- *~60 profiling rounds per year, ~320000 CPU hours*
- *~23 validation rounds, ~23000 CPU hours*
- https://g4cpt.fnal.gov

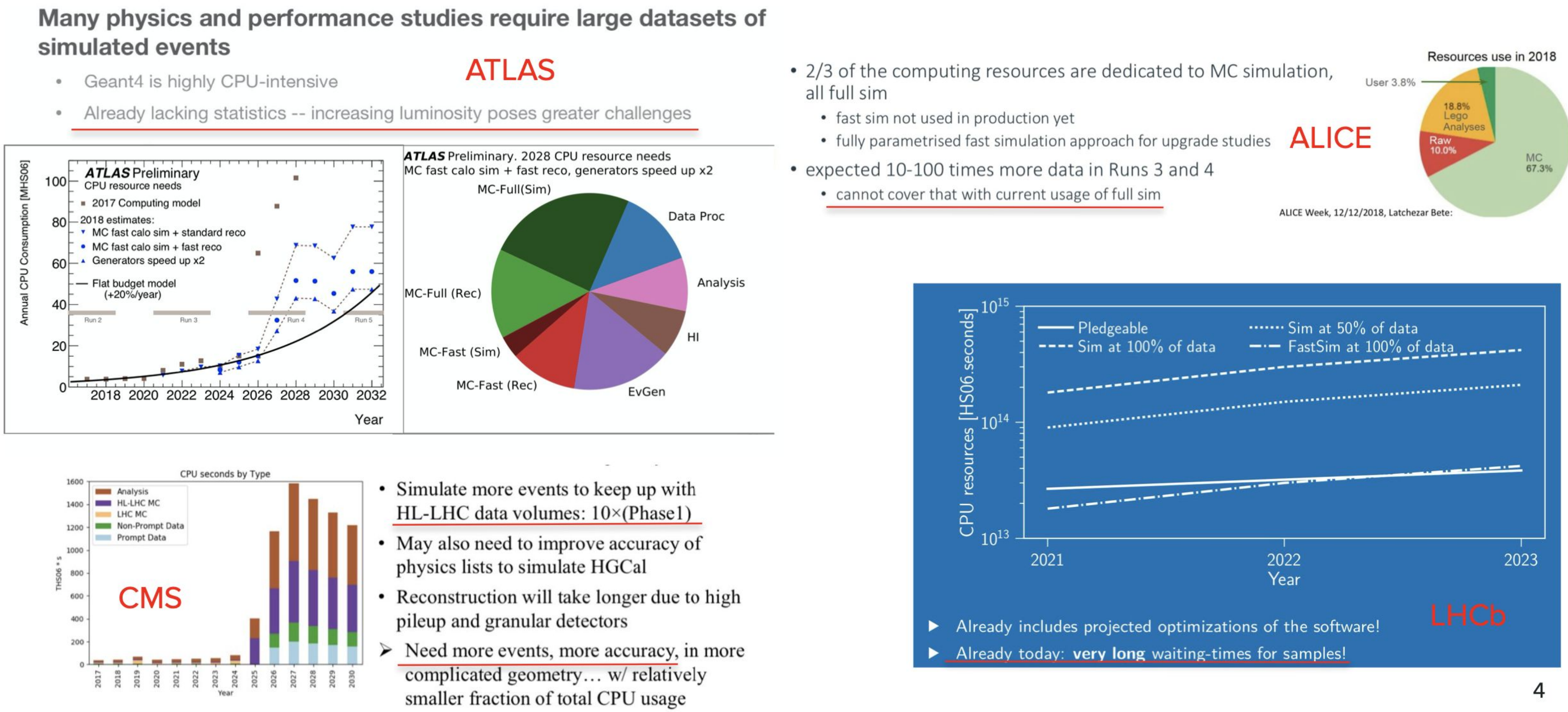
Maintaining Physics Precision and Performance

Dedicated Testing and Quality Assurance Working Group



https://g4cpt.fnal.gov

20% speedup from 9.6-10.0
Further speedups **plus** better physics accuracy



HL-LHC Needs on Simulation Performance

Don't forget Neutrino, Low Background, Beamlines. Some specific challenges/differences

Near/Longer Term Developments

- Near term modernization/optimization of Geant4
  - *Tasking framework*
  - *Physics/Geometry/Kernel algorithms*
  - *Code/data layout, call sequencing, reduce state*

- R&D on **tooling to assist fast simulation development**

- R&D on potential **use of accelerators** such as GPUs and/or FPGAs

Tasking Framework

- Pool of threads without predefined call stack
- “Tasks” ~ function calls placed on a queue
- Pooled threads idle until tasks pushed to queue
- No major API changes
- Potential for sub-Event parallelism
  - *E.g. each primary G4Track could be processed as a task*
- May be important for leveraging accelerators
  - *Thread pools for “CPU” and “Accelerator”*
  - *Offload suitable tasks to accelerator queue*
- ***On Geant4’s workplan for 2020/21***

Usage of VecGeom

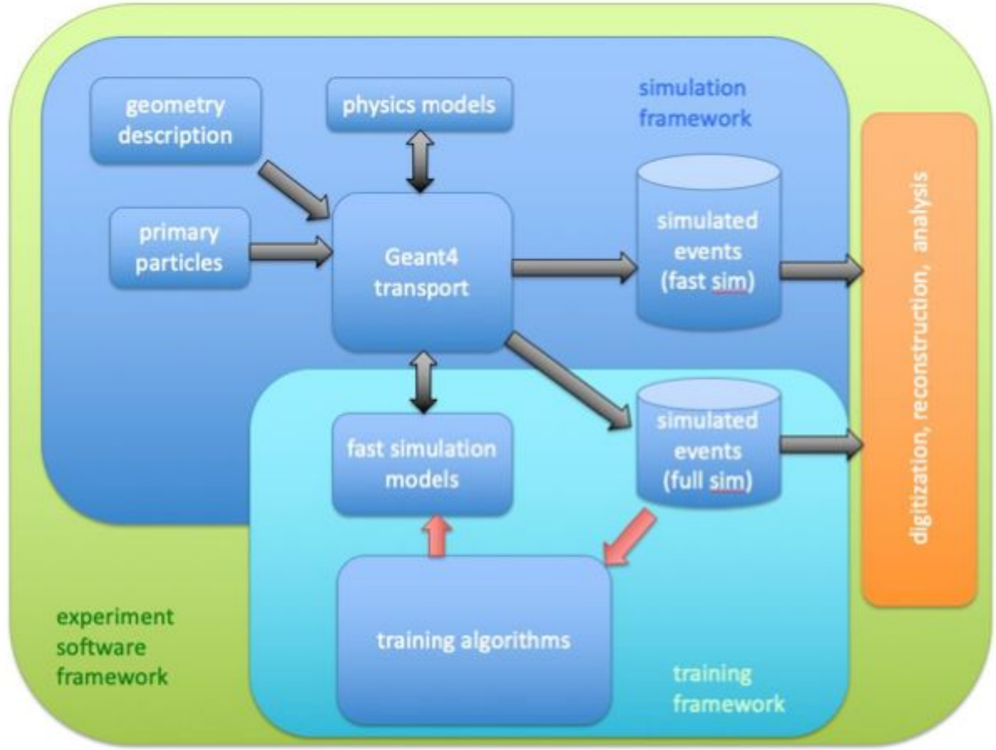
- Common library for HEP to describe geometry
  - *Improved scalar algorithms*
  - *Uses SIMD where possible*
  - *Shapes + distance/containment algorithms*
  - *Modelling + navigation: "ray tracing"*
- VecGeom **Shapes** as optional feature in Geant4 since 10.4, planned to become **production default in 2020**
  - *7-13(2-4)% speedup in CMS(ATLAS)*
- VecGeom **Navigation** as **optional feature (Beta version) in Geant4's 2020 release**

Refactoring Transportation

- A core process in Geant4, navigates particles through geometry and fields
- Only one transportation in memory, and handles all particle types (neutral/charged/photons)
    - *Results in frequent if/else branches*
    - *… On charge to decide on field computation*
    - *… On type to compute group velocity*
- **Study underway on transportation per-type**
    - *One each for neutral/charged particles*
    - *Eventually one for optical photons*
    - *Reduces branching and redundant calls*

Integrating Full/ Fast Simulation

- "Fast" (non-stepping) methods essential at HL-LHC to gain statistics
- Geant4's fast/biasing hooks allow easy integration of models **once developed**
- R&D on tooling/methods to assist users develop or train their experiment dependent models



R&D on Use of Accelerators

- Full simulation not a natural candidate for GPUs/FPGAs
  - *Few localized hotspots*
  - *Many branches, special cases, large data tables*
  - *Work unknown in advance (Monte Carlo!)*
- *Some* success for limited use cases over the past 5-7 years
  - *Low-Energy EM in simple geometries, Neutron/Optical Photon transport*
- Portability, usability, flexibility, sustainability **must** be retained
  - *Otherwise any gains could easily be lost in maintenance/support*
- *Accelerators are here to stay for the near future though, so where might benefits be found for full simulation?*

Existing Studies with Accelerators

- MPEXS, MPEXS-DNA for radiotherapy/biology
    - *Voxelized phantom and single material only, only e-/e+/g at energies up to ~100MeV*
- GATE for PET/CT applications
    - *Voxelized phantom only, very limited set of EM processes at low energies*
- Opticks for optical photons using NVidia OptiX
    - *"Offload" photon processes/tracing to GPU, plus handlers for ray tracing with CSG/binary tree geometries (GDML)*
- Project at ORNL studying thermal and colder neutron transport with tessellated geometries
- ***Highlight many of the challenges involved with general Monte Carlo on accelerators***

Potential Accelerator R&D Explorations

- Geant4 work on Tasking, Transportation, Geometry
  - *Providing enhancements to users **right now** in addition to steps in reducing issues for Accelerators such as branching*
  - *Tasking may be important in "offloading" work*
- Further exploration of Neutron/Optical Photon transport
- EM physics at higher energies in restricted volumes
- VecGeom navigation and algorithms such as ray tracing
- APIs such as oneAPI/Alpaka/Kokkos for portability/sustainability
- See Geant4 R&D Task Force Meetings for more
  - *https://indico.cern.ch/category/11208/*

Summary

- Geant4 the primary full simulation toolkit for HEP
- *Architectural, performance, and physics enhancements delivered to experiments over >20 years*
- Near and longer term developments plus R&D underway on performance enhancements
  - *Geant4 work on kernel tasking, transportation, geometry, important stepping stone to future enhancements*
  - *Task Force for R&Ds on longer term work, inc accelerators*
  - ***Whilst maintaining physics accuracy, usability, and sustainability for experiments over the coming decade***