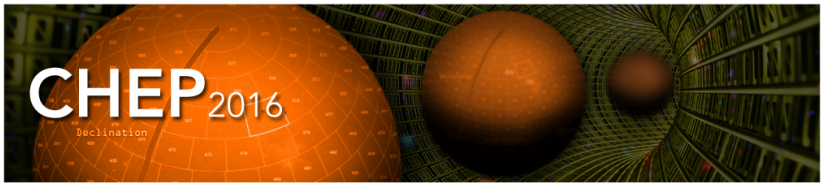

22nd International Conference on Computing in High Energy and Nuclear Physics, Hosted by SLAC and LBNL, Fall 2016

Geant 4

New Developments in Geant4 Version 10 Series

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On behalf of the Geant4 Collaboration

SLAC NATIONAL ACCELERATOR LABORATORY

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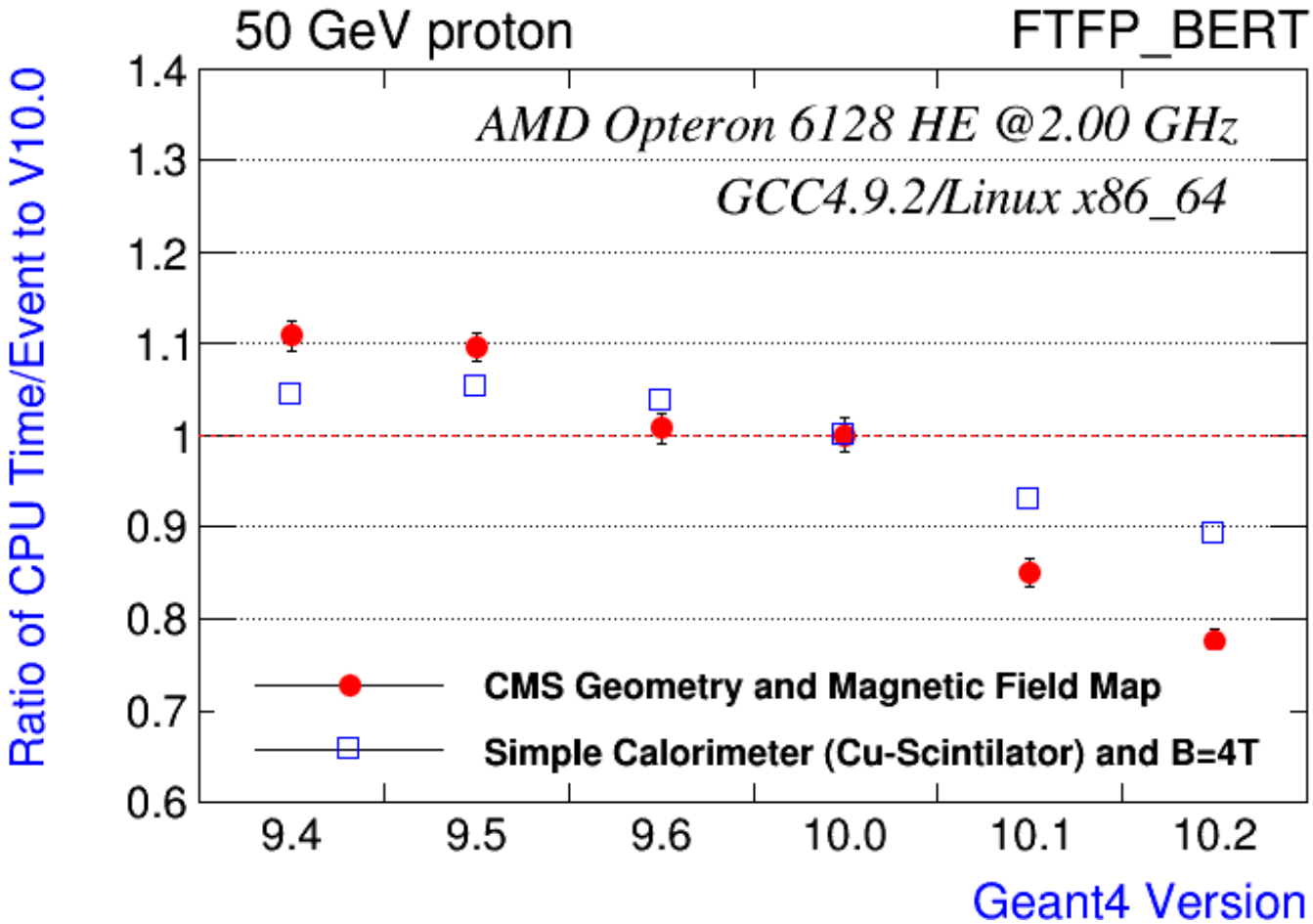
Geant4 Version 10 Series

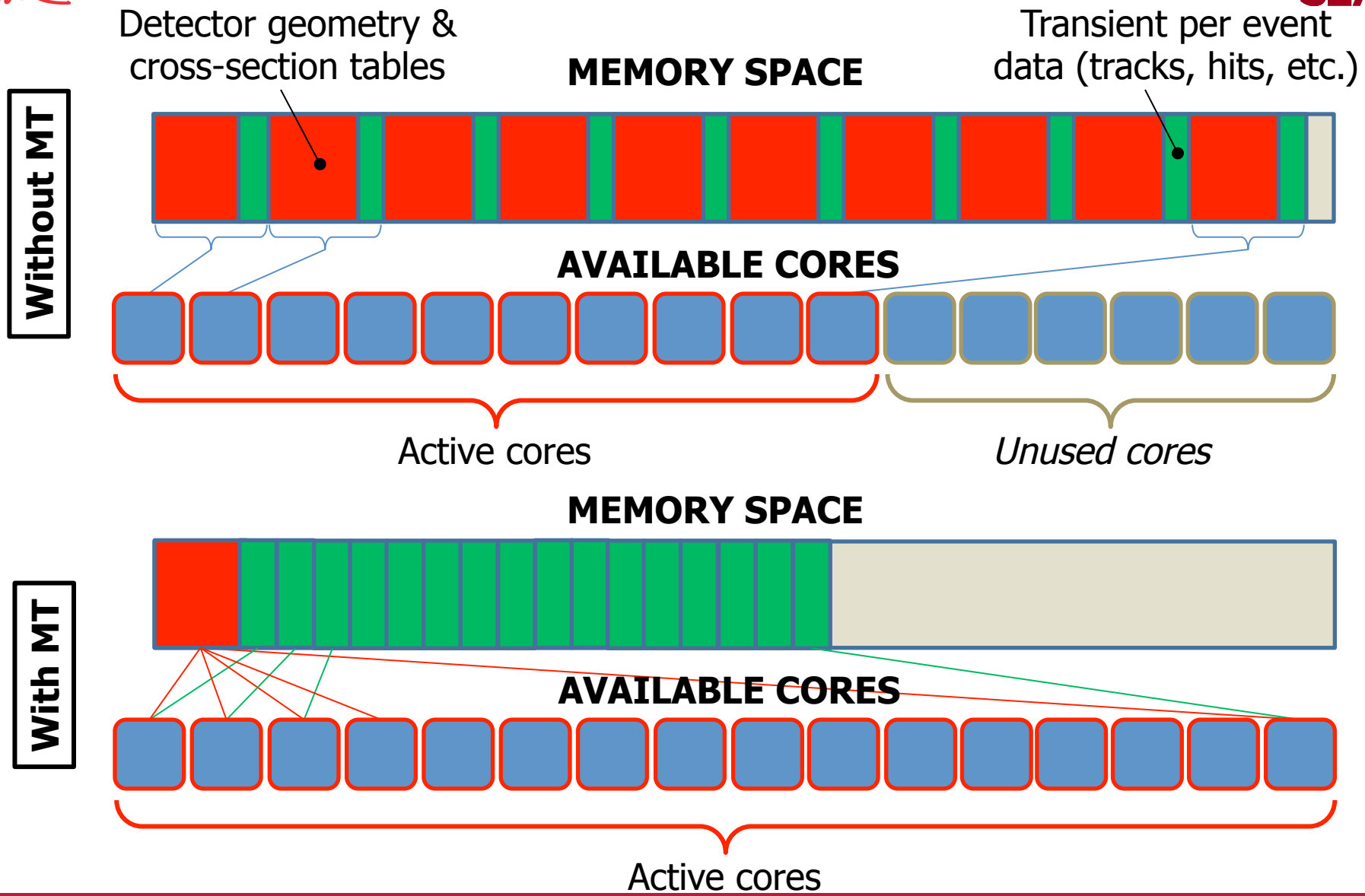
- Geant4 version 10.0 was released on December 6th, 2013.
  - The first major release since June 2007.
  - One of highlights was its multithreading capability.
  - Many users have successfully migrated to version 10 series and started to use it in multithreaded mode.
    - E.g. CMS : production v10.0p02-seq, development v10.2.p02-MT
  - Detail of version 10 is fully described in our third general paper.
    - J. Allison *et al*., "Recent Developments in Geant4", NIM A 835 (2016) 186-225
- Since the 10.0 release, the Collaboration continues its efforts to improve the performance in both physics and computing, enrich the functionalities and offer user support.
- In this presentation, we will introduce recent developments in version 10 series.

First of all, we are making it faster!



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

Memory usage in multithreaded mode



More memory-efficient, more HPC friendly

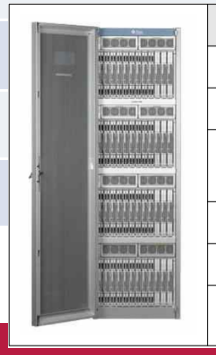
Version	Intercept	Memory/thread
9.6 (seq.)	113 MB	(113 MB)
10.0.p02-seq	170 MB	(170 MB)
10.0.p02-MT	151 MB	28 MB
10.3.beta-MT	148 MB	9 MB

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%
80	640	626	97. 8%
160	1280	1251	97. 7%
320	2560	2297	89. 7%
640	5120	3555	69. 4%

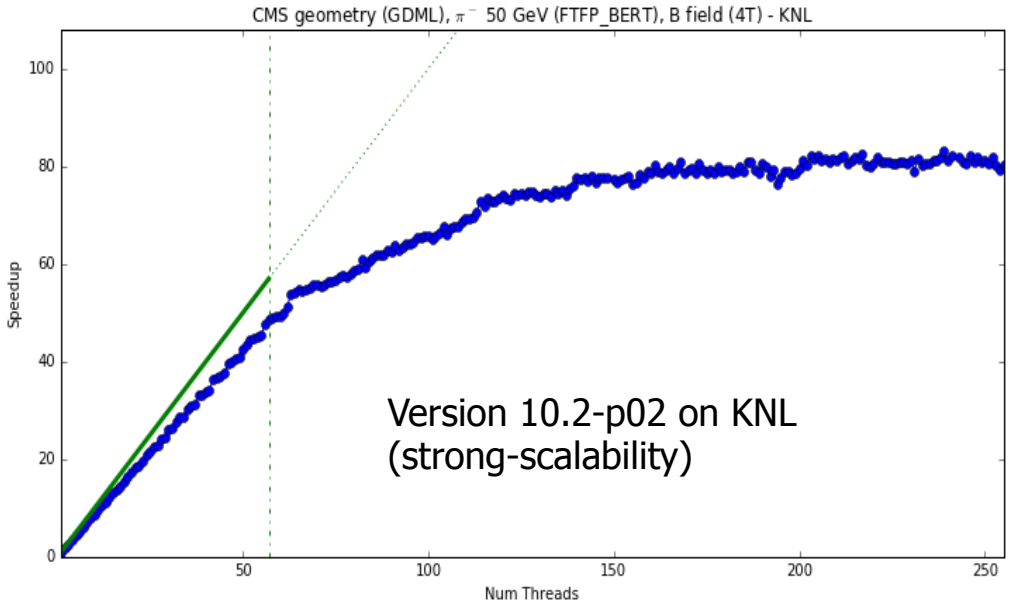
Tachyon-2 supercomputer @ KISTI (South Korea)
FTFP_BERT physics validation benchmark

- Geant4 has successfully run with a combination of MT and MPI on Mira Bluegene/Q Supercomputer (@ANL) with up to ¼ million threads
  - Full-CMS geometry & field
- I/O is the limiting factor to scale above 128k concurrent threads:
  - Granular input data files, output data/histograms, etc.
  - 2016/2017 work item



Section	Specs.
Model	SUN Blade 6275
Blade Nodes	3176 Compute Nodes, 300 TFlops (Rpeak)
CPU	Intel Xeon x5570 Nehalem 2.93GHz, 8 cores per node, Total 25408 cores
Memory	24 GB (per node)
Storage	1125 TB (Disk) 2112 TB (Tape)
Interconnect Network	Infiniband 4x QDR

Many core, many thread

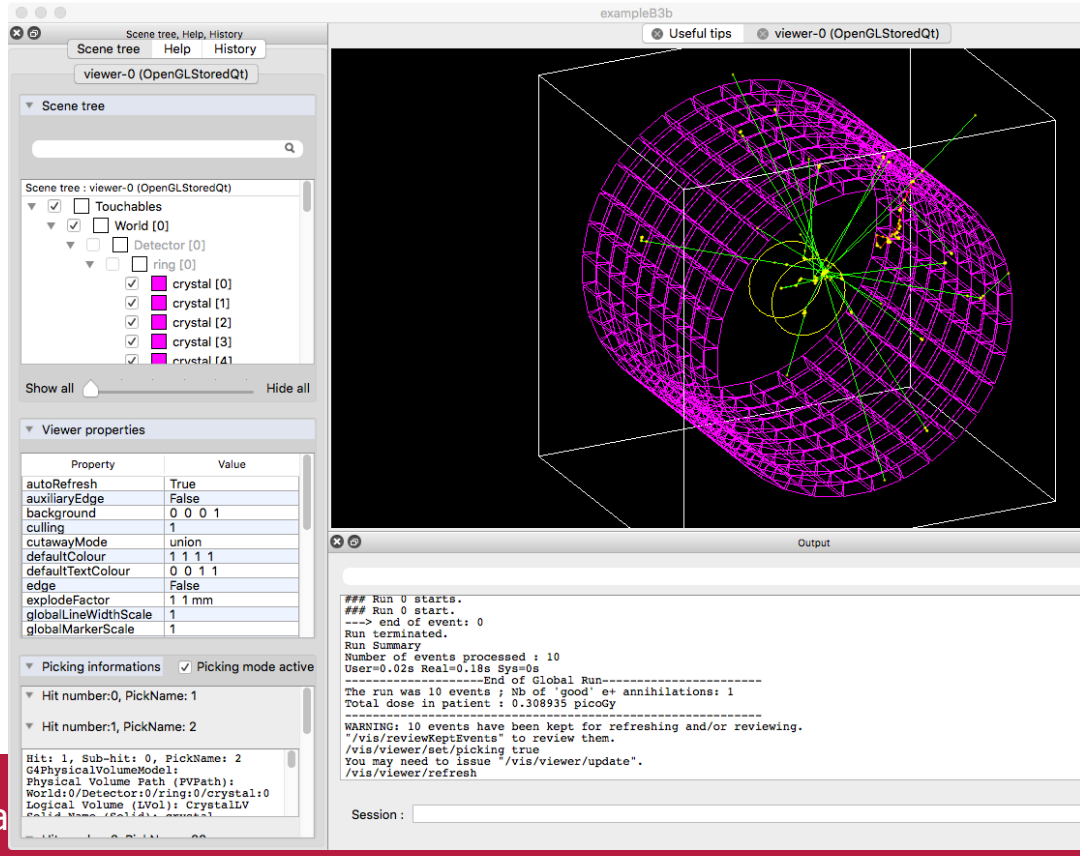


- For two years we have provided support for running Geant4 on KNC. We will soon extend our support to KNL.
- With KNL, thanks to x86 binary compatibility including the use of gcc, work-flow is tremendously simplified.

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)

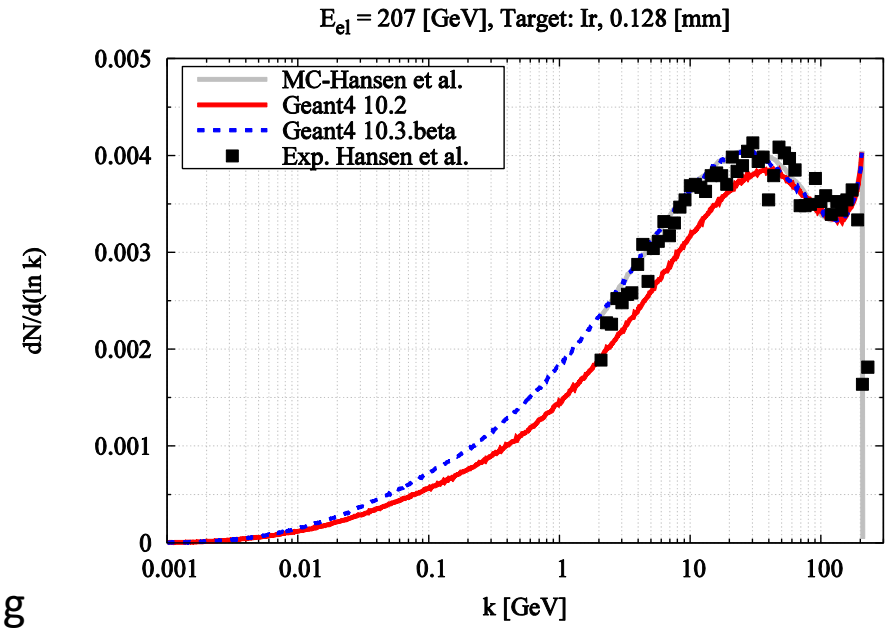
Geometry and transportation

- Parameterization by solid types and divided volumes are enabled in MT mode.
  - Last remaining incompatibilities were removed!
- Calculation of solid extent is being fully revised for most relevant shapes. This brought more efficient geometry optimization for navigation (“smart voxelization”).
- New ability to scale shapes along Cartesian axes (G4ScaledSolid).
- New magnetic field steppers (integrators) implementing third and fifth order Runge-Kutta.
- *VecGeom* solids can be used as an external library.
  - Work as alternatives to many Geant4 solid shapes.
    - Ability to choose individual shapes to replace at Geant4 installation phase
  - More advanced implementation, better computing performance
  - Supposed to be in production quality by 10.3 release



EM physics

- Implementation of LPM suppression in e± bremsstrahlung is fully revised.
  - Better agreement with CERN and SLAC experimental data
- Upper energy limit is extended from 10 TeV to 100 TeV.
  - Essential for FCC R&D
- Goudsmit-Saunderson multiple-scattering model is revised.
  - Angular distribution as well as computing performance are improved.



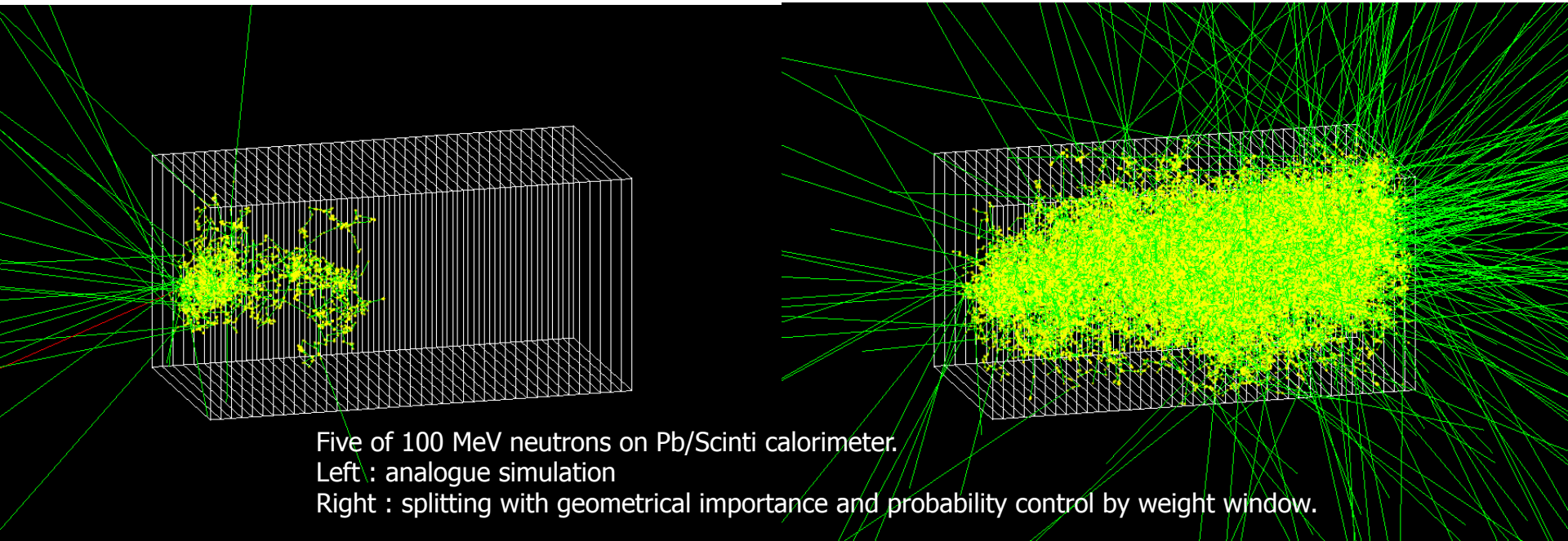
- New direct e+e- pair production process by e±
- Easier handling of EM model parameters and options
  - All EM model parameters are centrally managed by the new G4EmParameters class and configurable through its access methods or corresponding UI commands.
  - EM physics options can be configurable per each G4Region.

Hadronic physics

- All models are revised for better physics quality and/or computing performance
  - String models for hadron-nucleus and nucleus-nucleus collisions at higher energies (few Gev ~ few TeV)
    - Fritiof (FTF) model and Quark Gluon String (QGS) model
  - Intra-nuclear cascade models for intermediate energies (few hundreds MeV ~ few GeV)
    - Bertini-like (BERT) model, Binary Cascade (BIC) model, Liege cascade (INCL) model
  - Pre-compound and de-excitation models for lower energies
- Radioactive decay process is fully revised with more consistent and precise modeling, extended physics coverage (more rare decays and heavier elements), production of isomers (meta-stable nuclides), and better biasing capabilities.
  - Growing interest from Luminosity Frontier and nuclear physics experiments
- Neutron_HP is extended to Particle_HP to include proton, deuteron, triton, He3 and alpha below 200 MeV

New biasing scheme

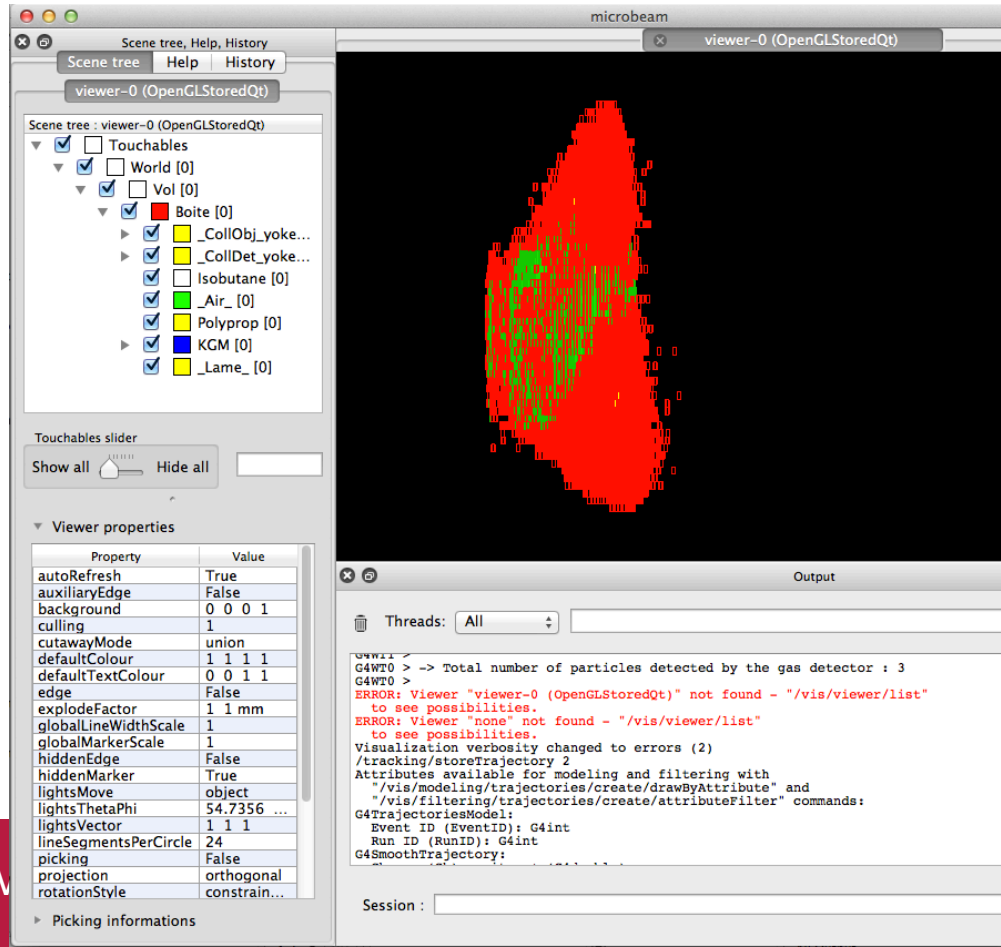
- Event biasing (a.k.a. variance reduction) scheme has been fully revised at version 10.
  - It allows treating many biasing options in coherent manner.
- Such options include:
  - Physics process biasing : alters physics process
    - Cross-section biasing, forced interaction, forced passage, etc.
    - 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 (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 by weight window.

New features in analysis, GUI and visualization

- New built-in fully-multithreaded histogramming tool
  - 1-D and 2-D histograms and scatter plots (auto-reduction in MT mode)
    - Data format compatible with ROOT, XML, AIDA, CSV
    - Extensible to other formats
  - Parallel n-tuple writing in ROOT format in MT/MPI mode
- Job control by macro commands
  - If-statement, loop commands
  - Simple arithmetic
  - Access to Unix environments
- 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



More detail talks and posters

- Oral presentations
  - Tuesday AM Track #2
    - J.Yarba *et al.*, "Software Toolkit to Study Systematic Uncertainties of the Physics Models of the Geant4 Simulation Package"
  - Tuesday PM Track #5
    - A.Dotti *et al.*, "Multi-threaded Geant4 on Intel Many Integrated Core architectures"
- Posters
  - Poster-A (Tuesday)
    - I.Hrivnacova *et al.*, "Analysis Tools in Geant4 10.2"
  - Poster-B (Thursday)
    - D.Sawkey *et al.*, "Recent Progress of Geant4 Electromagnetic Physics for LHC and Other Applications"
    - E.Bagli *et al.*, "Simulation of Orientational Coherent Effects via Geant4"
    - A.Dotti *et al.*, "Software Aspects of the Geant4 Validation Repository"
- There also are many presentations/posters by users.

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.
- 2014 was the 20th anniversary 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 large-scale physics software in the world.
  - Next evolution is migration to the recent C++ standards, C++11/14, that enables us to better manage threads and memories used by threads.
  - New physics models for coming experiments, e.g. hadronic model for multi-TeV regime (for LHC run-II/III/IV), specialized EM model for noble liquid (e.g. liq.Xe) and neutrino physics model (for intensity frontier)
- Geant4 is nowadays mission-critical for many users including all HEP experiments, space missions, medical applications, etc. Geant4 will be maintained and continue to evolve for at least next decade.