The Geant4 Toolkit: Evolution and Status

John Apostolakis & Makoto Asai for the Geant4 Collaboration
Outline

• Geant4 introduction and Application Areas

• New kernel capabilities

• Physics model improvement, tuning
  – EM Physics – new models
  – Hadronic Physics model improvement

• Computing Performance and Multi-core

• In each case, only highlights are shown
  – These slides can be found at http://bit.ly/g4mc2010
Geant4 Introduction

Application Domains
A tour of tools based on Geant4
Geant4 toolkit on one slide

- Mature, extensible kernel
  - Powerful geometry modeler, E/B fields, track stacking
- Diverse set Physics models (mostly 2 alternatives)
  - e-/e+/gamma 10s eV to TeV
  - Hadron-nucleus interactions up to 1 TeV
  - Neutron interactions from thermal to 1 TeV
  - Ion-ion interaction from 100s MeV/n to 10 GeV/n
  - Optical, weak (decay of unstable and radioactivity)
- Tools for input, output, visualization, scripting
- Every increasing use
- Product of collaboration of 90 contributors
  - Effort: HEP (75%), Biology/medical (15-20%), space (5-10%).
High Energy Physics Experiments
Space: radiation effects, science

Akebono, RHESSI, ACE, LISA Pathfinder, INTEGRAL, GLAST, SOHO, Herschel, Cassini, Bepi Colombo, Messenger, GAIA, Kaguya, Suzaku, EJSM, XMM-Newton, CoreXpress, Chandrayaan-1, ISS Columbus, EUSO, AMS, MAXI, Simbol-X, Chang'e-1, LRO.
Geant4 @ Medical Science

• Four major use cases
  – Beam therapy
  – Brachytherapy
  – Imaging
  – Cell Irradiation study
Application Areas

• Established as the leading tool for the simulation of detector response for High Energy Physics (HEP) experiments
  – Used at ATLAS, CMS and LHCb as the production simulation (the fourth large LHC experiment is preparing to use it in production)
  – Used in a large number of smaller experiments, in nuclear physics, dark matter searches, ..

• Widely used in medical applications
  – Radiotherapy (external and brachytherapy)
  – Medical imaging

• **Space**
  – Satellite electronics radiation assessment
  – Planetary science applications.
Tools based on Geant4 (sample)

Medical physics
- **GATE**
  - Tomography/dosimetry*
  - Widely used, cited.
- Tools for radiotherapy
  - PTSim
  - Hadrontherapy
  - **GAMOS**
    Each is presented in E5 (Wed)

Accelerator beamline:
- **G4BEAMLINE**
- **BDS-SIM**

Medical phys., accelerators

- **HEP:** “Version1” of Detectors
  - **SLIC**
- Space radiation and environment tools
  - **GRAS** (radiation analysis)
  - **Planetocosmics** (planet environment),
  - **SPENVIS**
  - **CRÈME-MC**
  - **MULASSIS** (shielding)
Geant4 Physics

A lightning update
EM Physics
Multiple Scattering

• Many model refinements
  – See EM talk*
• Converged on unified design for EM models
  – Anyone can combine models for a process
  – Choosing ‘best’ of lowE and Standard packages.
• Validation extended
  – Suite of 15 tests and over 200 thin-target cases
  – Regular regression cross-checks for EM calorimeter performance

*Talk by V. Ivantchenko (Session I2, Wednesday 16:00-18:30)

Improvement of MS
– New step limitation
– Greater stability
• Benchmarking PBM paper
• Models tuned for e-, p, μ

Geant4 Toolkit, S

[Graph showing dose simulation/theor comparison]
Hadronic Physics

- FTF, CHIPS models improved, extended
  - FTF now works down to 3 GeV (overlap with cascade), improved and retuned
    - Details in talk of V. Uzhinskiy (moved to J2 - Thursday)
  - CHIPS: new model for hadron-nucleus interactions.
- Bertini cascade: improved pion cross-sections
  - Poster PB #16
- Improvement in elastic, quasi-elastic interactions
  - New quasi-elastic at high energy (CHIPS for QGS, FTF)
  - Improved cross sections for elastic scattering
- Improved Pre-compound / de-excitation
  - Precompound: revised cross-sections, transition
  - SMM corrections (from original authors)
  - Mix simple and GEM evaporation
    - Details is talk of J.M. Quesada (previous talk- was J2 session)
Ion-ion interactions

• ‘Previous’, older models
  – **Binary** light-ion cascade (BLIC)
    • E<10 GeV/A; projectiles: C or lighter
  – Abrasion / ablation

• New Interface to **DPMJET 2.5**
  – Created for space applications (funded by ESA)

• New native **QMD** model (G4QMD)
  – Borrows from JQMD
    • nucleus creation method and potential
  – Uses scatterer of Binary cascade
    • See talk by T. Koi (J1 - earlier)

*G4 QMD reaction*

*Fe 290MeV/n on Al*
Example of evolution of production physics lists

- **LHEP**
- **QGSP (2003)**
- **QGSP_BERT (2007)**
  - Adds Bertini cascade
  - Ongoing improvements
    - Revised Mult. Scatt. (G4 8.1, Jun 2006)
    - Improved quasi-elastic (G4 8.3, May 07)
    - Revised elastic (‘08)

- **FTFP_BERT**
  - FTF extension down to 3 GeV (2009)
  - Is not the leading *alternative* to QGSP_BERT

Production physics lists for HEP Applications

Geant4 Toolkit, SNA-MC 2010
Kernel developments

Improved ‘parallel’ geometries
New scoring, via UI commands
Propagating tracks back in time
Parallel geometries

• Joint navigation in two or more geometries
  – Step is limited by first boundary found

• Many uses in toolkit already
  – Materials (‘mass’ geometry) – used for physics
  – Scoring / tallying
  – Importance biasing and weight window
  – Shower parameterization (and other fast simulation)

• Engineered flexible framework – open to additional uses
  – By developers of tools, advanced applications
New Scoring via scripting

- Scoring redesigned,
  - Tallies for does, energy deposition, fluence, ...
- Driven by interactive commands or scripts:
  - Start/stop of scoring
  - Choice of quantities
  - Location, orientation of meshes
- Uses parallel geometry capability
- Scoring via user-defined hits is still possible
Reverse Monte Carlo

- Tracks e-/gamma/proton back in time
  - from sensitive target volume
  - to an extended source(s).
- Adjoint MC*
  - Continuous gain of energy
  - Multiple scattering
  - Discrete ionisation, bremsstrahlung, Compton, photo-electric
- Test cases show 5-15% accuracy
  - 100-500 faster for small target.
- Alternative, ‘simple’ reversal
  - With propagation of error matrices
  - For track reconstruction (HEP).

*Thanks to Tom Jordan

Results for electron exp(-E/2MeV) spectrum

Geant4 Toolkit, SNA-MC 2010
Other toolkit elements

- Expanded visualisation
  - Trajectories “a-la-carte”
  - Hooks to track attributes
- Interactive/GUI-driven environment
  - to explore detector, hits
  - Choice of simple (OpenGL) or full featured interface
    - Joint Qt driver for viz/UI
- Input of geometry description from CAD
  - Tools to translate to GDML, tesselated solids
    - Commercial FASTrad tool (from TRAD)
Trajectories ‘a-la-carte’

Creator Process
- muIoni
- Decay
- annihil
- eIoni
- brem

Charge
- +1
- 0
- -1

Momentum (MeV)
- 0-1
- 1-10
- 10-20
- 20-30
- 30-50
- 50+
Computing Performance

“Driving” Applications
Improvements
Multi-core
Computing Performance - Context

Computing performance is a significant issue for many communities of users

- Big HEP experiments make large productions
  - Running on 10k CPUs many months each year

- Medical dose estimation need turnaround time
  - accuracy needs => significant statistics
  - use complicated geometries (CT)

- Few sacrifices in physics modeling accepted
  - Need the ‘best’ physics modeling
  - In addition to “as-fast-as-possible” computation

- Backdrop: hardware is now many-core computers
Performance Improvement

- Measured measure CPU time & number of memory allocation
  - Tools: standard (valgrind, perfmon2) and custom (igprof, FAST)
  - Undertaken in close collaboration with key user communities
- Eliminated hotspots and frequent causes memory allocation:
  - Improvements in Bertini cascade (30%), EM Low Energy (25%), step integration in magnetic field (15%), geometry (5-10%).
  - Several improvements (not all) relevant for typical use cases.
- Eased the cost of improved physics modeling in large scale productions (e.g. use of Bertini cascade in HEP.)
  - Afterwards the CPU-time cost has returned to the cost with older versions of the simpler, less precise modeling
    - e.g. parameterised models for E<~18 GeV, as in QGSP physics list
Improvements for voxel geometries

• Navigation in a regular grid of voxels is greatly improved
  – No longer is there a penalty of large memory use.
• New option to ignore boundaries between voxels with the same material and density
  – Real speedups for new “Regular” navigation
    • e.g. of 4 in CT-scan test case with 57 “materials” by skipping boundaries (vs previous ‘Nested’ method).
    • P. Arce IEEE/NSS 2008
• Alternative methods of gluing volume in GATE

<table>
<thead>
<tr>
<th>CPU time spent on tracking 1000 geantinos</th>
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<tbody>
<tr>
<td>Vx 1-D</td>
</tr>
<tr>
<td>--------</td>
</tr>
<tr>
<td>2030</td>
</tr>
</tbody>
</table>
Parallelism and multi-core

Older efforts / New era
- Distributed-memory Parallel Geant4 (v1=2000)
  - ParGeant4 developed and released (2002) - joint output
- New issue: reduce memory use
  - Multi-process/copy-on-write
    - 70 MB extra/worker (vs. baseline 250MB)
  - Multi-threading
    - Big task – not in original design

Multi-thread prototype
- Developed prototype multi-threaded Geant4
  - shares the physics tables and geometry
  - 20MB added per thread
  - 95% efficiency on 32 cores,
    - Bottlenecks fixed in memory allocation, creation of new ion.
- Today’s Challenge:
  - Whether/how to incorporate into code repository.
Summary

• Several Physics model improvements
  – EM physics from 10s eV to TeV
  – Hadron-nucleus models up to TeVs.
• Improved Computing Performance
  – Multi-core alternatives investigated
• IMPACT - Very wide use in diverse fields
  – Many tools based on G4 for diverse fields
• Flexibility, Open Source enable many uses