# GEANT4: Release 6.2 Update

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# Outline

- Relevant developments until December 2003 (G4 release 6.0)
- Highlights of developments, improvements and fixes in
  - Kernel
  - Physics Processes
  - Physics Lists
  - in releases 6.1 (Mar 2003) and 6.2 (June 2004)
- Geant4's use in production
  - Improvements to help identify problems
  - Performance

#### Notes:

# For more information see <u>http://cern.ch/geant4/</u>
# for full details the release notes at <u>http://cern.ch/geant4/source/</u>
# only some individual attributions mentioned

## Geant4 6.0 - general picture

- New capabilities in Geant4 6.0 for HEP

   # EM ('standard') : new 'model' implementation
   # Hadronic physics lists ported & included
- 2. Numerous improvements
  - **#** to existing physics modeling & models;
  - **#** in physics process implementations;
  - **#** extending functionality that existed
- 3. Fixes, improvements, refinements
  - **#** Resulting from the high level of user feedback
    - **#** which is reflected in many developments, fixes & improvements

#### Focus of 6.x releases

- Release 6.0 included
  - New physics models
  - Integrated solutions
    - Physics list for hadronic use cases
  - Redesigned / revised implementations
    - EM (std)
  - Refined functionality
  - Interface changes

- Release 6.1 (Mar 04)
  - Stability improvements
    - For production
  - New tools to identify production issues
  - Fixes / improvements
- Release 6.2 (Mar 04)
  - Additional models
  - Performance focus

The high level of user feedback is reflected in developments, fixes & improvements

#### Part I: The 'Kernel'

New developments & improvements in Geometry, Tracking, Run & Event handling

#### Kernel: summary 6.0/6.2

#### Development

- Modular Run Manager
- Better HEPMC input
- Abstract Navigator
- New Biasing
  - Biasing:"weight-window" technique

#### Refinements

- General Particle Source
  - Design iteration
- Integration of motion in field
  - Enabled tuning of accuracy parameters
     for particle type, Energy, ...

#### Improvements Navigator:

- New 'check mode'
- better verbosity

#### Fixes

- Corrected 'safety' in solids
  - Addressed propagation & photon problems
    - Reported by LHCb
- Fixes for case of missed intersections in field
  - purging magnet example
  - Fixes for a 'point outside' problem seen in solids
    - problem in displacement in field

# Kernel: Geometry

- Protections & actions for stuck tracks
  - New check in G4Navigator counts zero steps
  - Actions taken:
    - After 10 does corrective action
    - After 25 abandons event
- Improved verbosity for checking when navigating
  - 'Check' mode, combined with verbose level=1, prints more information
    - To help identify issues in user geometry or in navigation
- Reflection of division volumes
  - Experiment request
- Solids:
  - Framework for twisted solids (derived/refined)
  - New G4TwistedTubs shape

O. Link

I. Hrivnacova



View of Atlas toroid Courtesy of Atlas



J Apostolakis for G4 Collaboration & G4/SFT team

### Kernel: Identifying geometry issues

- It is easy to create *overlapping* volumes
  - During tracking Geant4 has not performed check for malformed geometries
- Added new ability to perform checks of the navigation & model geometry (J.Apostolakis & G.Cosmo)
  - New 'check mode'
    - Available unless G4\_NO\_VERBOSE environment variable is set when compiling the Geant4 installation
  - More message to aid users/developers in identifying issue

Note: The full problem of detecting 'significant' *overlaps* is now addressed by the specialised tools:

- Commands for verification (DC Williams; G Cosmo)
- DAVID intersects graphics volumes (S. Tanaka)
- Example with full navigation (M Liendl)



Thanks to S. Tanaka

# Kernel 6.2: Hits & Events

#### • Digitization & Hits

- G4SDManager, G4SDStructure: added optional argument *warning* to FindSensitiveDetector(pathName, warning), defaulted to true, to eventually exclude warning issued by G4SDManager when sensitive detector is not found.
- Event
  - Design iteration of the G4GeneralParticleSource class:
    - New classes have been added. See <u>http://reat.space.qinetiq.com/gps</u> for more details of the changes.
    - New formula for converting integral spectrum to differential one.
  - G4EventManager:
    - Added access methods to G4TrackingManager and G4StackManager.
    - Fixed incorrect behaviour of event abortion requested by BeginOfEventAction().

### Part II: Physics

Using the Physics & & Physics modelling

# Tailored Physics 'lists'

- "Educated guess" physics lists are for direct use, or as a starting point to modify.
- Revised with experience of comparisons with data
  - Provide 'tested' options, with known performance;
  - The same package is tested for different detector technologies.
- Physics lists for hadronic use-cases updated with
  - New physics models of Geant4 6.0
  - Experience from comparisons (eg Jan-Mar 2004)
  - Latest updates in March 2004 for Geant4 6.0; June for 6.1 / 6.2
- New module for use cases of 'standard' electromagnetic physics
  - Module includes sample physics lists for these standard EM use cases.
- Distribution
  - Included in Geant4 releases
    - Hadronic since Geant4 6.0 (Dec 2003) ported version for major release
    - Current physics lists version is included in minor releases, patches.
  - Most up-to-date from the G4 hadronic physics web pages <u>http://cmsdoc.cern.ch/~hpw/GHAD/HomePage</u>

## EM Physics Processes (6.0)

- New "model-based" EM standard physics processes are now the default (since 6.0)
  - for maintaining and refining
  - keeping user code unchanged
    - Old (frozen) implementation is still available
  - Issues encountered in transition
    - Fixed in 6.0 patch 1 and 6.1
- Fix for reproducibility issue
  - Multiple scattering does not use tables (due to ions)

- Refinements
  - Tail of multiple scat. angular distribution
- New in Low Energy EM
  - New models (2BN, 2BS) for Bremstrahlung (Lisbon & INFN)
  - New processes for electrons & positrons (a-la Penelope)

#### EM Physics Processes ( 6.1 & more)

#### • Multiple scattering

- Tuning for tail of angular distribution
- Improvement for muons of E>1 PeV
- Ionization
  - Updated energy intervals, fluctuation models ...
  - Multiple scattering does not use table
    - Needed to ensure repeatability
  - Added PAI (Photon-Absorption-Ionisation) model
- Optical processes
  - New process for wavelength shifting
  - Adoption of G4SurfaceProperty class for materials
- Fixed problem reports
  - ionisation in air with low pressure less than 10-4 Atm;
  - in simulation of fluctuation of energy losses in very small steps (performance issue, from ALICE).



# EM Physics: 'Standard' / 6.2

- Improvements in Multiple Scattering (MS) model
  - Changed true to geometrical length conversion (& reverse)
    - Meant to reduce step size dependence due to low energy MS
  - Expected to affect the resolution of sampling calorimeters
- Use 'integral method' for μ, ion & hadron ionisation (as e<sup>-</sup>)
  - New default still limits step to 20% current range (as in G4 5.2)
- Improved Sampling in Integral methods
  - For processes whose cross-sections have peaks
- Energy loss fluctuations
  - For very small steps, modified to reduce step-dependence in results
  - Smoothed sampling of Gaussian fluctuations, when  $\sigma_E > E_{loss}$

## EM 'Standard' 6.2 (cont)

- New, second, Photo Absoption Ionisation (PAI) model
  - Splits the cross section between electrons and photons
- Updated
  - calculation of radiative corrections
    - for Bethe-Bloch model for muon energy above 1 GeV.
  - parameterization for  $\mu \rightarrow e^+ e^-$  model in region E > 100 GeV

# Electromagnetic Processes (Low-energy)

- New models for PIXE
- Photoelectric angular distribution: redesign, with reimplementation of Sauter-Gavrila distr.
- Fix in positron energy loss process (
   'Penelope' variant )

#### Hadronic Physics: Extensions & Improvements / 6.0

- Added biasing in framework
  - leading particle biasing for any reaction
  - cross-section biasing for e-/N and  $\gamma$ /N reactions
- Binary cascade:
  - included pion projectiles
  - added light ion reactions
  - improved transition to pre-equilibrium model
- Bertini Cascade
  - improved in the range 5-10 GeV
  - verified its suitability for isotope production estimation
- QGSM string model: improved meson splitting
- Improved selection of element for creating final state

# Hadronics: improvements in 6.1

#### • Identifying initial conditions in crashes & other problems

- White-board and Signal-handler prints the reaction conditions.
  - Also run-time checking the energies of all secondaries for NaN values.

#### • Improvement of CHIPS (Chiral invariant Phase Space) model

- Big upgrade of the CHIPS nuclear fragmentation model: more hyperons are added to fragmentation algorithm
- New conservation, step by step, of energy/momentum and charge/baryon number
  - Fixed issues identified.
- Fixes
  - 'Logic' fixes, eg for suspended particles
  - Fixed a few memory leaks and for occasional non-conservation scenarios
- Refinements
  - Introduced minimal transverse mass for diffractive scattering of gammas.
  - Updated implementation of  $\mu$ -nuclear absorption at rest.

#### Hadronic processes Technical issues (6.1 and 6.2)

- Identifying problem conditions (6.1)
  - Added white-board, signal handler and C++ exceptions
    - That record initial reaction conditions and print them out in case of 'soft' error or program crash
  - As a result problems can be fixed faster
    - Instead of needing 2-5 days to reproduce, can be found in an hour.
      - Turnaround time for a fix is much faster, even for rare problems.
- Particle ID after interaction
  - Optionally kill primaries (LHCb request)
    - can be steered from user code
- Fixes for reported problems

#### Hadronic Models: new & improved in 6.2

- Evaporation models
  - *Ablation*: new model for use with abrasion code
  - GEM model implementation
  - HETC emission probabilities for Weisskopf-Ewing evaporation model
- Ion Reactions
  - Wilson's Abrasion for induced ion reactions.
  - *EM dissociation* for ion-ion collisions
- High energy elastic scattering: new coherent elastic model
  - requires a tabulation, which is kept as a 'data set' (provided)
- Diverse
  - new  $\mu^{-}$  nuclear absorption code
  - Improved fast radioactive decay code
  - GNASH2 transition probabilities now available
    - in exciton precompound model

#### Hadronics: Cross Sections & Scattering

- Cross sections:
  - Newest pion scattering data of 'Barashenkov'
    - remove discontinuities
  - Fix in high energy p-H cross-sections (G3 legacy bug)
  - Ion-ion cross-sections
    - Tripathi's systematics for ion-ion cross-sections for light ions
    - Parameterizations from Shiver, Kox and Shen
- Scattering term
  - extended for nucleon induced reactions to 8 GeV
  - included s-wave absorption
  - pion induced reactions (up to 1.5 GeV)

### Hadronics: Improvements & fixes

Element selection in creating final state

 fix for materials with many elements
 now choosing isotope before calling model
 using A<sup>2/3</sup> cross-section approximation

#### Hadronic Processes Summary of changes in 6.2

- New packages and models:
  - *Ablation*: model for evaporation (for use with abrasion code).
  - *Abrasion*: package for ion reactions.
  - EM dissociation.
  - *Coherent elastic*: new model for high energy elastic scattering, requiring a new provided data set for elastic scattering data.
- Cross sections:
  - Removed discontinuities in pion scattering data.
  - Fix in high energy p-H cross-sections (G3 legacy bug).
- Particle ID after interaction
  - Optional kill primaries can be steered from user code (LHCb request)
- Fixes for reported problems

### Part III: Auxiliary

User Interaction Performance 'Platforms'

## User Interactivity

- Visualization
  - Ported OpenInventor driver to Windows
    - And revised, so as not to depend on HEPVis
  - Renamed 'zlib' prefix to 'heprep\_z'
    - To resolve conflict with other programs/libraries with zlib
- Environments
  - New version of MOMO Java tools
    - MOMO included in distribution (since 6.0) includes
      - GGE (Geometry editor)
      - GPE (Physics editor)
    - New version of GPE includes change/fix.



## 'Platform' changes

- Enabled loading of dynamic libraries
  - Shared library mechanism
  - Targeted for Windows
    - Request of LHCb
  - Also usable on
    - MacOS 10.3
- Newly supported (June 2004)
  - gcc 3.2.3 on Linux
    - Red Hat 7.3 and SLC 3
  - Visual C++ .net 7.1
    - on Windows XP

- 'Higher' Optimization level
  - -O2 is new default (for gcc)
    - in place of -O (ie –O1)
- OS / compilers verified
  - Emerging platforms
    - MacOs 10.3 with gcc 3.3
    - icc 8.0 (IA-32 & IA-64)
  - Check for porting
    - Latest gcc: now 3.4
- Dropped / Dropping
  - egcs already
    - end-2003
  - gcc 2.95.2 & Vis C++ 6
    - end-2004

### Allocator and Dependencies

#### G4Allocator

- Added utility methods
  - to de-allocate storage
  - to print total pages
- Under user control & responsibility

#### AIDA

- Examples moved to AIDA 3.2.1
  - Many use PI implementation

#### CLHEP

- G4 6.2 requires CLHEP 1.8.1.0
- Moved development to 1.9.1.1 (beta)
  - Works since September (ref-03)
    - Thanks to CLHEP team
    - Await public release!!
  - For now, still works with 1.8.1.0
- Geant4 7.0
  - See next slide

## Geant4 7.0 and 'dependencies'

- For Geant4 7.0 evaluated/ing impact of potential moves to:
  - <cmath> (agreed)
  - CLHEP 2.0 (under discussion)
  - <sstring> (postponed full move)
- Concern for use of CLHEP 2.0, focused on
  - Usability of long units names
    - Clhep::units::GeV
    - Compromise of clhep::GeV is still seen as 'bulky'
  - Impact of move on user communities is unclear

## CPU Performance (condensed)

- Our geometry benchmarks
  - demonstrate that the geometry is as good or faster (simple or complex cases)
- Performance in several experimental setups (with Geant4 releases 2 and 3) was comparable to Geant3
  - A few counterexamples, including BTeV ECAL.
  - New issues arose in Geant4 4.0
    - and nearly all were addressed (in patches & release 4.1)
- Difficult cases remain, including
  - Some setups of EM showers (particularly large blocks)
  - Field propagation in complex setups (eg CMS), factor  $\sim 2x$  which are under active investigation.
- Collecting a set of benchmarks
  - To follow computing performance regularly
- Goal is that Geant4 is at least as fast as Geant3 in almost all cases
  - When comparisons are made for configurations that obtain the same physics performance.
    - And, of course, when its power is used adequately

## **CPU** Performance

- Performance in several experimental setups
  - Issues raised in 2002: BTeV ECAL, Atlas EMB,
    - Slowdown typically 2.0x 3.0x compared to Geant 3.21
    - Degradation from Geant4 3.2
      - Issues in Geant4 4.0 were resolved (in patches & release 4.1)
    - Improvements lead to typical factor ~1.8x vs G3 (eg EMB, Sep 02)
- In 2003/4 the most difficult cases included
  - Some setups of EM showers (eg large blocks "no geometry")
  - Field propagation in complex setups (eg CMS), factor  $\sim 2x$
- Performance improvements obtained
  - About 20% better (CMS) with 5.2
    - Key areas identified: EM & propagation in fields





Using Composite Calorimeter. Source R Yaari

20 October 2004

**B=0** 

80%

60%

40%

20%

0%-

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#### Performance: status & actions



# CPU 'Benchmark' suite

- Benchmark suite created
  - Simple setup(s)
    - Started from Extended TestEm2
  - Test beam(s)
    - LHC experiment calorimeter(s)
  - Magnetic field
    - derived from simplified BaBar setup
- Benchmarks in regular use
   used to check dev-tag performance

## New example applications

#### Contributed by partners

- Cosmic ray charging from LISA (ESA)
- Hadron therapy
- Medical linac
- *Purging magnet* (S Larson, Karolinska)
- Radio protection
- LXe: Optical (TRIUMF)
- Parallel: ExDiane (CERN & INFN)
   Revised 3 EM(std) 'extended' examples

   Added check for automating regression tests

#### Part IV: Past 6.2 / Future

Regression testing 'Migrations' in 7.0 Upcoming features

#### Patches for release 6.2

- Patch 1 (July 2004)
  - Fix for multiple scattering
    - Particles above 80 GeV suffered large deflections in thin media
- Patch 2 (upcoming)
  - Fix for problem with switching materials in parameterized volumes
  - Fix for problem report in Bertini cascade (HARP)

# Statistical testing 2003/4

#### • Establishment of 'statistical testing' suite

- Automated comparison of physics quantities
  - Against 'standard' data (eg NIST)
    - INFN and SLAC efforts
  - Reusing donated 'test-beam' comparisons
    - Full applications from ATLAS, CMS.
  - Simple setups for 'regression testing'
    - Simplified, typical HEP detectors without digitisation
  - For details see A Ribon's talk in G4 Workshop 2004 (soon)
- Note also the established benchmark suite for computing performance
  - Simple and test-beam setups

## Kernel Changes for 7.0

Several changes in kernel are planned for the 7.0 release. A number will impact users

In order of the effects:

- New scheme of storing/retrieving physics tables
  - Enables user to read a portion & generate the rest
- New "unknown" particle and "unknown decay" process
  - For particles whose physics is not simulated, we now create
  - Enables full decay chains to be treated uniformly
- New dedicated class/process for user step limitation
  - Separating step length limitation from track killing
- Possibility to alter detector sensitivity with the parameterized volume
- For process writers, new methods in Particle Change
  - Eg SetEnergyChange becomes ProposeEnergy
  - New UI commands for G4GeneralParticleSource

#### Established new releases & new features

- Established releases
  - End of June (minor release)
  - End of December (major release)
- The activities planned in 2004
  - taking into consideration requirements of all users including those from LHC experiments / LCG

# Requirements and Releases

- Geant4 Users' Technical Forum <a href="http://cern.ch/geant4/technical\_forum">http://cern.ch/geant4/technical\_forum</a>
  - Requirements collection and first-level prioritization
  - Quarterly meetings, next ones: 4<sup>th</sup> Oct (Catania), 16<sup>th</sup> Nov (CERN).
- Upcoming developments and releases
  - 2004 work items & planned release contents
    - At URL <a href="http://cern.ch/geant4/source/planned\_features.html">http://cern.ch/geant4/source/planned\_features.html</a>
    - Started from requirements and requests of users/experiments
  - Next major release Geant4 7.0 in mid-December
    - New developments
    - Improvements and other refinements
    - Changes that require interface changes
    - Any fixes, further performance improvements.
- Developments available
  - In monthly development tags
  - In open  $\beta$  releases each quarter
    - If there are relevant developments, not included a minor or major release.

### Feedback and improvements

Much feedback received from users, partners:
On physics validation

LCG, ATLAS, CMS, BaBar, GLAST, HARP.

Extensive pre-production tests

CMS, ATLAS and LHCb (2003-04)

Large scale and emerging production

Enabled and assists in identifying open issues.

# Challenges / Ongoing

- Identifying 'unwanted' changes
  - Towards an 'acceptance' suite
    - Regression tests for automated testing
    - In addition to user/experiment acceptance tests
- Performance improvement
  - Large productions / always a goal
- Expanding use of 'best-practice'
  - Eg new methods to identify 'hard' problems

#### http://cern.ch/geant4

# Summary

- Geant4 latest minor releases 6.1 and 6.2 included
  - Refinements and new features in the kernel
    - Allocator features; navigator
  - New models, improvements & refinements in EM
    - Improving the new 'model-based' implementation
    - Reducing memory footprint
  - Extensions, improvements & new models in hadronics
    - Also leading particle & cross section biasing
  - Revisions for hadronic physics lists & new EM (std) lists
- \_Geant4 is evolving
  - With experience in experiment production and use in medical, space and other application domains.
  - Much, excellent, feedback from LHC experiments, BaBar in 2003/4
  - Users' Technical Forum meetings for discussing requirements and priorities