LCG Application Area 2005 Review, 31 March 2005

Physics Validation and recent development in Geant4 and Fluka



Physics Validation

Outline

- Goals
- Strategy
- Results since the last review
- Work plan and resources

For more information

http://lcgapp.cern.ch/project/simu/validation/

Project Goals

- Compare Geant4 and Fluka with the LHC test-beam data;
- Test coherence of results across experiments and sub-detector technologies;
- Study simple benchmarks relevant to LHC;
- "Certify" that simulation packages and framework are ok for LHC physics;
- Weaknesses and strengths of the packages.

Strategy

- As for the choice of the Geant4 Physics List, the validation should be targeted to each considered application domain: e.g. for high-energy physics one should consider different observables than, for instance, medical physics, or space science.
- The criteria to consider a simulation "good" or "bad" should be based on the particular application: e.g., for LHC experiments, the main requirement is that the dominant systematic uncertainties for all physics analyses should not be due to the imperfect simulation.



Validation setups

Two main types of test-beam setups:

1. Calorimeters: the typical test-beams (made mainly for detector purposes).

The observables are the convolution of many effects and interactions. In other words, one gets a macroscopic test.

- Simple benchmarks: typical thin-target setups with simple geometry (made, very often, for validation purposes).
 It is possible to test at microscopic level a single interaction or effect.
- These two kinds of setups provide complementary information

Results

- We consider here the main results on the Physics Validation project since the last review in October 2003 (about one year and a half).
- Fabiola Gianotti has been the coordinator from the beginning of the project until September 2004.
- First cycle of electromagnetic physics validation completed at the percent level. We will focus here only on the hadronic physics validation.



Double-differential neutron production (p,xn)

Proton beam energies: 113, 256, 597, 800 MeV

Neutron detectors (TOF, scintillators) at 5 angles

Study of the neutron production spectrum (kinetic energy) at fixed angles.

Pion absorption - experiments

Witold Pokorski CERN-LCGAPP-2004-11



•Nakai – look for gammas emitted after pion absorption

• Ashery – look for transmitted (not absorbed) pions

π[±] beams of energies between 23 – 315 MeV

Absorption X section for π^+





- both G4 and Fluka show reasonable agreement
- in some cases Fluka seems to be a bit better
- difficult to make more conclusions because of big uncertainties in the experimental data

Absorption X section for $\pi^{\scriptscriptstyle -}$





- same remarks as for pi+
- for heavy material (Au) the shape of the QGSP_BERT quite different
- G4: best agreement for 'medium-weight' materials

Hadronic interactions in ATLAS pixel test-beam



Geant4 Geometry. Use the same Geometry also with Fluka, using FLUGG (interface between the Transportation and Physics of Fluka and Geant4 Navigation of the Geometry).

Number of reconstructed tracks



Pseudorapidity distribution



Ratio max Eloss / total Eloss



QGSP is in excellent agreement with data.

Cluster size



QGSP produces too narrow clusters. FLUKA, LHEP and QGSC are in good agreement with data.



In conclusion, FLUKA, Geant4 are in reasonable good agreement with the data, but some observables can be improved.

LHC hadronic calorimeter test-beams

F.Gianotti et. al CERN-LCGAPP-2004-10

AILAS:

HEC : copper + LAr HEC1 + HEC2, 4 longitudinal compartments 6-150 GeV for electrons; 10-200 GeV for charged pions; 120, 150, 180 GeV for muons.
Tilecal : iron + scintillator tile 2 extended barrel + 1 barrel + barrel 0 modules 20-180 GeV electrons and charged pions; 1, 2, 3, 5, 9 GeV charged pions.

CMS:

 combined ECAL + HCAL : ECAL : prototype of 7 x 7 PbWO4 crystals HCAL : copper + scintillator tile each tile is read out independently Max magnetic field of 3 T 10-300 GeV muons, electrons, and hadrons.

Calorimeter test-beams CMS HCAL & ECAL



ATLAS HEC



Alberto Ribon, Carry and a

43 40 ĊВ

30 30

32

29 30

57

41 42

89 +5. +5 лιο

47

energy resolution of pions

 $\left(\frac{\sigma}{\langle E \rangle}\right)_{test-beam}$ $\left(\frac{\sigma}{\langle E \rangle}\right)_{simulation}$



 e/π ratio

$\left(\frac{e}{\pi}\right)_{simulation} / \left(\frac{e}{\pi}\right)_{test-beam}$







<u>CMS longitudinal shower profile in HCAL for 100 GeV pions</u>



Radiation studies with Geant4

Background radiation studies for LHC experiments have been done mainly with Fluka . It is very interesting to compare them with Geant4, which offers a precise treatment of low energy neutrons with some Physics Lists like QGSP_BERT_HP.

- Giuseppe Daquino (LCG) is working on radiation studies for LHCb: preliminary results have been already presented, and comparisons with Fluka will be ready by the end of April.
- Pedro Arce (CMS) is working on similar radiation studies for CMS.

- Summary of the results Monthly meetings, talks accessible from the Web page: ٠ http://lcgapp.cern.ch/project/simu/validation/
- Presentations of results in various conferences (e.g. ACATO3, IEEE-2003, CALOR-2004, CLHEP04, etc.)
- Results documented in LCGAPP notes:
- ✓ J.Beringer, CERN-LCGAPP-2003-18, "(p,xn) Production Cross Sections".
- ✓ A. De Roeck et al, CERN-LCGAPP-2004-02, "Simulation Physics Requirements from the LHC experiments".
- ✓ A. Ribon, CERN-LCGAPP-2004-09, "Validation of G4 and Fluka Hadronic Physics with Pixels test-beam data".
- ✓ F. Gianotti et al, CERN-LCGAPP-2004-10, "G4 Hadronic Physics Validation with LHC test-beam data: First Conclusions".
- ✓ W. Pokorski, CERN-LCGAPP-2004-11, "In-flight Pion Absorption: Second Benchmark Study for the Validation of Hadronic Physics Simulation".

Proposed work plan for 2005

- New LHC test-beam results (e.g. ATLAS combined; CMS): second half of the year;
- Checks of the longitudinal shower shape with Geant4 7.0 : first half of the year;
- Geant4 background radiation studies for LHCb and CMS: first half of the year;
- Simple benchmark test: inclusive charged pion production (multiplicity, y, p_T) in π[±], K⁺, p, pbar interactions on Mg, Ag, Au, at 100 GeV/c: middle of the year;
- Extension to Fluka for at least one calorimeter test-beam setup: second half of the year.

Current LCG man power

- G. Daquino : 75% F.T.E. dedicated to LHCb radiation studies with Geant4. Leaving at the end of April.
- M. Gallas : 75% F.T.E. dedicated mainly to ATLAS Combined Test-Beam, and some support for the ATLAS calorimeter test beam setups.
- W. Pokorski : 30% F.T.E. dedicated to simple benchmarks, and extension to Fluka of the calorimeter test beam setups.
- A. Ribon : 50% F.T.E. dedicated to coordination, simple benchmarks, and extension to Fluka of the calorimeter test beam setups.

Possible work items beyond 2005

- Analysis of relevant LHC test-beams that have not yet been used for Physics Validation;
- New simple benchmark tests;
- Collection (e.g. database + Web interface) of data useful for detector simulation validation (similar to JetWeb for Event Generators);
- Try to transform the LHC test-beam setups into stand-alone setups to be used for Geant4 validation at each release;
- Systematic procedure for tunings/validation of simulation codes (both Event Generators and detector simulation engines).

Physics Validation Summary

- A lot of work has been done in the last year and a half, concluding a first round of hadronic physics validation, with good results.
- For Geant4 hadronic physics, calorimeter energy resolution and e/π are well reproduced by Physics Lists QGSP and LHEP. For shower shapes, further work is needed and it is currently undergoing.
- For this year, new test beam results, and further comparisons Geant4/Fluka on radiation studies, calorimetry, and simple benchmark are expected.
- There are still many useful and important things that remain to be done in the coming years.

II part

Geant4

(transparancies provided by John Apostolakis)

Geant4 in production

- Three LHC experiments (ATLAS, CMS, LHCb) now using it successfully in production
 - OSCAR (CMS), Gauss (LHCb) and ATLAS's G4-based simulation programs are the production tools.
 - OSCAR and Gauss have replaced G3 based simulation
 - Substantial productions (numbers from Oct 20th Aplic. Area meet. presentations)
 - ATLAS DC2 (summer 2004) produced 12M events
 - Oscar (CMS): 35 M pp interaction events, and first 100 Pb-Pb events
 - Gauss (LHCb): Over 200 M events simulated
 - Production use demonstrated low crash rate (and decreasing with new releases)
 - Rate decreasing from 1/10K events (5.2, CMS) to 1 per Million events (6.1, LHCb)
 - G4 team addressed issues found in test productions
- The Geant4 LCG/SI sub-project and the Geant4 Collaboration
 - LCG/SI/G4 responsible for CERN/LHC participation in Geant4
 - Work plan integrated with overall Geant4 plan
 - Geometry and tracking in field, Physics: hadronic and electromagnetic, testing and release, coordination

Geant4: 2004 goals

- Feb 2004 Savannah/SPI prototype portal for problem reporting system for Geant4
 Prototype and assessment delivered; under evaluation in the Geant4 Collaboration
- Mar 2004 Release 6.1 (Contributions in several areas)
 - focused on improving production usage in LHC experiments
- Jun 2004 Scheduled release 6.2 (Contributions)
 - focused on better use of computing resources, including performance and memory use, and refinements to specific physics models, persistency and windows support
- Sep 2004 Development release
 - included additional geometry volume registration, refinements to physics models
 - supported CLHEP 1.9, and still compatible with CLHEP 1.8
- Oct 2004 First consolidated acceptance suite for LHC applications
 - Suite of simplified test-beam setups created, and being deployed
- Dec 2004 Release 7.0 (Contributions)
 - Release 7.0 contributions focus on improvement of physics models and additional geometry functionality
- Dec 2004 Prototypes & Process Improvements
 - prototype 3D string fragmentation; ensure maintenance and improve examples, system tests and physics lists
- Dec 2004 Geant4 validation in LHC production (added May 2004)
 - documenting results, response to feedback, status of production use of Geant4

Geant4: some highlights

- Geant4 reliability in production: crash rate low and decreasing
 - CMS (Geant4 5.2, 1 crash per 10,000 events)
 - ATLAS (Geant4 6.0 patch1, ~1 crash per 1 Million events)
 - LHCb (Geant4 6.1, ~1-2 crashes per 1 Million events)
- Support and maintenance
 - Addressing issues found in LHC experiment production
 - providing high job 'robustness' (less than ~1 per mille job failures in 6.1, 6.2)
- Code improvements to help identify problem conditions
 - In hadronics and geometry (Geant4, releases 6.0 & 6.1)
- Creation of 'statistical testing' suite
 - Automated physics comparisons in simple test-beam-like setups
 - Deployed for validation of release 7.0 (December 2004)
 - Requires significant computer resources
- New and improved physics models
 - And improvements in EM & hadronics (Geant4, releases 6.1 & 6.2)
- Refinements & more functionality in kernel
 - E.g. enabling experiments to easily construct detectors, register volumes, ...
 - Reflections, divisions, ...
- New fast shower capability (a-la GFLASH)
 - Integrating efforts in LHC experiments into Geant4 toolkit
 - New addition, just scheduled for Geant4, release 7.0

Geant4: Key characteristics of latest releases

- Release 6.0 included
 - New EM implementation
 - Hadronic physics-lists
 - New physics models
 - More functionality
- Release 6.1 (Mar 04)
 - Stability improvements
 - For production
 - New tools to identify production issues

- Release 6.2 (Jun 2004)
 - Additional physics models
 - EM computing performance
- Release 7.0 (Dec 2004)
 - Compute Volume/Mass
 - Treat 'unknown' particles
 - Shower parameterisation
 - a la GFLASH, for 1 material

Geant4 Geometry

- Abstraction of G4Navigator
 - Also consolidation of the interface
- New Divisions volumes (with P. Arce, CIEMAT)
 - for slicing volume, offers more options Replicas (including offsets)

G4Box, G4Tubs, G4Cons, G4Para, G4Trd, G4Polyhedra, G4Polycone

- Solids:
 - Review of 'safety' in Boolean & CSG solids
 - Addressed issues from production, optics.
 - New twisted box & twisted trapezoid shapes
- Volume Registration
 - Added hook, called when one is created
 - Used in experiment framework (ATLAS)
- New abilities to compute volume, mass
- Propagation in field
 - Refinement of accuracy per field 'manager'

Geant4 Kernel

Design revision of Run-Manager Modular for experiment use (thanks to M. Asai) Eased maintenance & use in exp. frameworks Better save/restore of physics tables Can create & treat 'unknown' particles Geant4 to create tracks where physics is done already by event generator! Enables uniform treatment of track/trajectory

Shower parameterization

A shower parameterisation 'a-la-GFLASH'
 Implemented by members of ATLAS & CMS
 Adapted & released first implementation
 Single material part released in G4 7.0
 Thanks to J. Weng, A. Barberio

Future: sampling fractions for sampling calorimeters

Standard EM physics

New "model-based" EM standard physics processes are now the default

- model approach for energy loss and MSC
- we can more easily maintain and modify them
- to enable the easy use of different models for a single process (e.g. ionization) in one application
- previous user-interface unchanged
- Performance optimization for EM showers
 - Speedup for low production threshold ('cut') values
- Improvements in high Energy processes (above 10 TeV) :
 - Revision of muon Bremsstrahlung process
 - Revision of muon ionisation and e+e- pair production
- New class to access for cross-sections and dE/dx
 - Roughly equivalent to drmat in Geant3.21
- Revision of the Photo Absorption Ionization model

Geant4 Hadronic Physics

- Binary cascade:
 - Concluded inclusion of *pion projectiles* and light ion reactions
 - improved transition to pre-equilibrium model
- Bertini Cascade: extended up to 10 GeV (thanks to A Heikinen)
- Scattering term
 - extended for nucleon induced reactions to 8 GeV
 - included s-wave absorption
 - pion induced reactions (up to 1.5 Gev)
- New packages and models:
 - Abrasion/Ablation & EM dissociation for ions.
 - Coherent elastic model for high energy elastic scattering.
- 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

Geant4 Hadronics 'Infrastructure'

Recent improvements & extensions

Identify conditions leading to problems

- Retain information on reaction initial conditions
- On error, print it to provide information for users & developers
- Added biasing in framework
 - \blacksquare cross-section biasing for e-/N and γ /N
 - leading particle
- Selection of target element
 - Choosing isotope centrally before calling 'model'
 Using approximate A^{2/3} cross-section approximation
 - Enables models to create appropriate final state

Hadronic Physics Lists

- The latest physics lists included since 6.0
 - 6.0 ported from the best available in Dec 2003
 - Full validation against use cases undertaken 1Q2004
 - Updates released as required (eg March, April 2004)
 - And incorporated in Geant4 releases
- Physics lists and builders are used:
 - As is, compiled in a 'deployment' directory
 - Altered (or additional/customized version) by user/experiment, in own installation



Fluka

(transparancies provided by Alfredo Ferrari and Paola Sala)

Fluka development framework

- Regulated by the CERN-INFN Agreement (Dec. 2003, signed by CERN DG and approved by INFN Council) and by the Scientific Agreement of Feb. 2003
- Scientific management by the authors (A. Fassò, A. Ferrari, J. Ranft, P.R. Sala)
- Overall supervision by Fluka Coordinating Committee (G. Battistoni (chairman), E. Chiaveri, J. Harvey, J. Ranft, P.R. Sala)
- Fluka: joint CERN-INFN copyright 1989-2005
- Authorship recognition and protection
- Confirmation that use of unauthorized versions infringes the copyright and will be dealt with accordingly

Heavy ion development: examples

- Upgrade of high energy ionion generator to DPMJET-III
- Development and implementation of a model to describe Ion electromagnetic dissociation: critical for lead ion operation in LHC

Coloured dots: experiments Full Histo: FLUKA Dashed: Elecromagnetic dissociation contribution



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Improvements to Evaporation and test of activation at CERF

M.Brugger et al, Proc ICRS10



Activation: example of results

Isotope	$t_{1/2}$	Exp		STD FLUKA/Exp		NEW FLUKA/Exp	
		Bq/g \pm %		± %		\pm %	
Be 7	53.29d	0.205	24	0.096	34	1.070	30
Na 24	14.96h	0.513	4.3	0.278	8.6	0.406	13
K 43	22.30h	1.08	4.6	0.628	8.7	0.814	11
Ca~47	4.54d	0.098	25	0.424	44	(0.295	62)
Sc 44	3.93h	13.8	4.8	0.692	5.8	0.622	6.2
${\rm mSc}~44$	58.60h	6.51	7.1	1.372	8.1	1.233	8.6
Sc 46	83.79d	0.873	8.3	0.841	9.1	0.859	9.5
Sc 47	80.28h	6.57	8.2	0.970	9.7	1.050	13
Sc 48	43.67h	1.57	5.2	1.266	8.4	1.403	11
V 48	15.97d	8.97	3.1	1.464	3.8	1.354	4.8
Cr 48	21.56h	0.584	6.7	1.084	11	1.032	12
Cr 51	27.70d	15.1	12	1.261	13	1.231	13
Mn 54	312.12d	2.85	10	1.061	10	1.060	11
Co~55	17.53h	1.04	4.6	1.112	7.7	0.980	10
Co~56	77.27d	0.485	7.6	1.422	9.0	1.332	10
Co~57	271.79d	0.463	11	1.180	12	1.140	12
Co~58	70.82d	2.21	5.9	0.930	6.3	0.881	6.9
Ni 57	35.60h	3.52	4.5	1.477	6.5	1.412	8.2

Table 1: Stainless Steel, cooling times 1d 6h 28m, 17d 10h 39m

The Voxel Geometry

Allowes complicated 3-d voxel structures inside standard geometries.



The first application: GOLEM (human phantom) for FLUKA application in space radiation and in therapy

(data from Zankl and Wittmann 2001, GSF)

from a CT "whole body" scan of an adult male of 68.9 kg. 2.2 million voxels, each is 2x2x8 mm3 122 organs/tissues (8 different densities, composition Alberto Ribon, CERN/PTASE from ICRU report no. 44)

Another application of Voxel geometry in FLUKA

Description of Gran Sasso mountain to build FLUKA transport of muons (E>1 TeV) from VHE atmospheric showers down to the underground laboratory (TCARUS collaboration)

Origin: local topographical map and geological survey



Here: 1 voxel = $100 \times 100 \times 50 \text{ m}^3$

FLUGG

- Upgrade to geometry in Geant4 v6
- New installation procedure (from full FLUKA and Geant4 distributions)
- Application to ATLAS Pixel

The 2nd FLUKA Course Houston January05

> Special Course in Beijing Dec 04



Applications for LHC

FLUKA- newly established team in AB department in charge of:

- Beam heating calculations for LHC Radiation damage calculations for LHC •
- •
- Collimation system studies CNGS radioprotection calculations ٠
- •
- CNGS engineering calculations Code development (CERN contribution) •
- 2 staff + 5 fellows +1 associate

For recent studies/examples see the

V. Vlachoudis presentation in <u>http://www.fluka.org</u>

IR7 Simulations

- Dynamic FLUKA input generation from machine optics files
- Detailed description of about 20 prototypes
- Magnetic field maps: Analytic + 2D Interpolated
- Prototypes are replicated, rotated and translated.
- Adjust the collimators planes during runtime!
- Dynamic generation of the ARC
- Optics test: Tracking up to 5 σ , both vertical / horizontal, reproduce beta function



A virtual tour in IR7



The Cern to Gran Sasso v beam



Neutrino event spectra at Gran Sasso available from CNGS web page



