HEP usability

A collection of topics impacting the usability of Geant4 by HEP experiment

Mostly from experience of LHC experiments

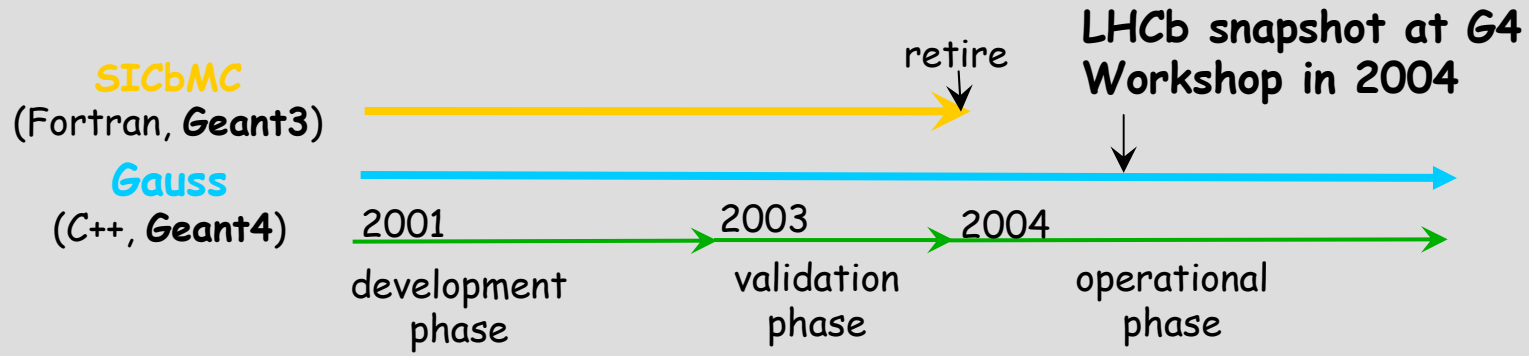
Time performance and tuning
Choosing settings and parameters
Robustness, stability and finding problems
(Migrating to) New releases and patches

Geant4 Review
16 – 20 April 2007

Gloria Corti
CERN/PH

Introduction

- **ATLAS, CMS and LHCb completed the migration of their simulation to OO applications using Geant4 in 2003-2004.**
  - **New applications had to be validated to replace existing Geant3 based software**

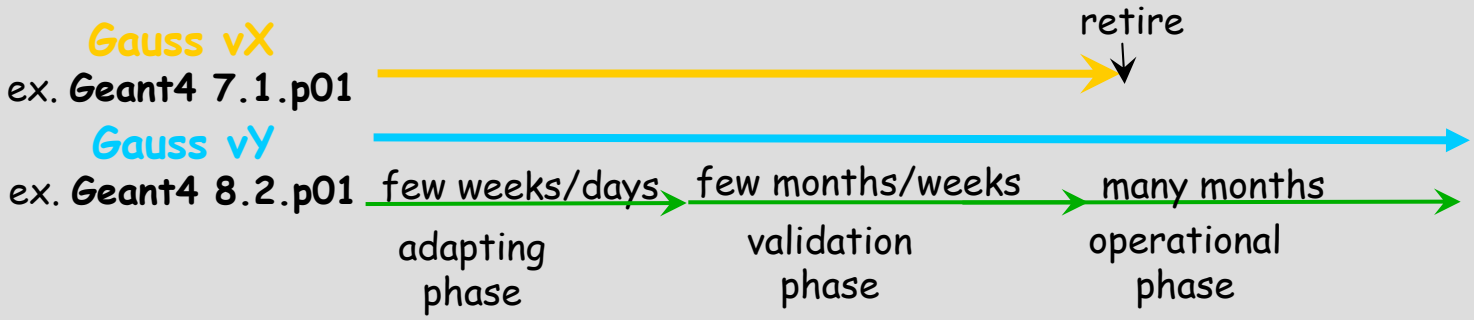


•Requirements for Gauss to be fully operational:

- complete
  - all detectors simulated
  - all information needed in later processing provided
- stable
  - low crash rate, reasonable CPU time
- validation of physics
  - comparison with the Geant 3 simulation (validation as replacement)
  - comparison with test beam data (tuning of physics setting)

Introduction

- **ATLAS, CMS and LHCb used Geant4 to produce hundred of millions of events in various Data Challenges**



•Requirements for new version of Geant4 to be fully operational in Gauss

- complete
  - any new necessary/desirable features introduced (e.g. detectors as built)
- stable
  - low crash rate, reasonable CPU time
- validation of physics
  - comparison with the previous version
  - comparison with (test beam) data

Adopting a new version

- **Now comparing with respect to previous version of Geant4**

- **ALICE is in the integration/validation phase of their Geant4 VCM**

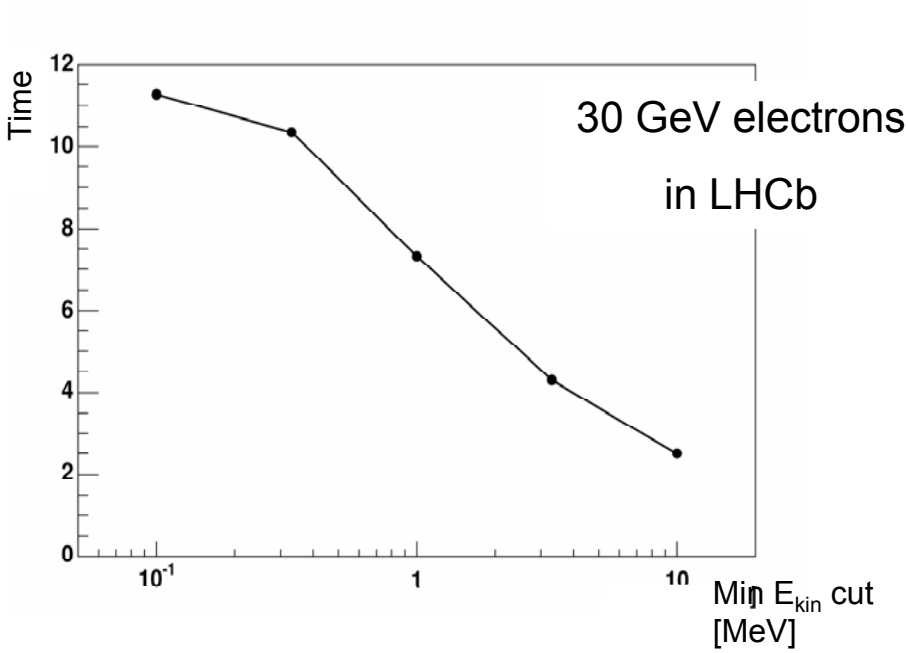
Time performance

Performance of simulation main component determining computing resources in term of CPU necessary for the experiments

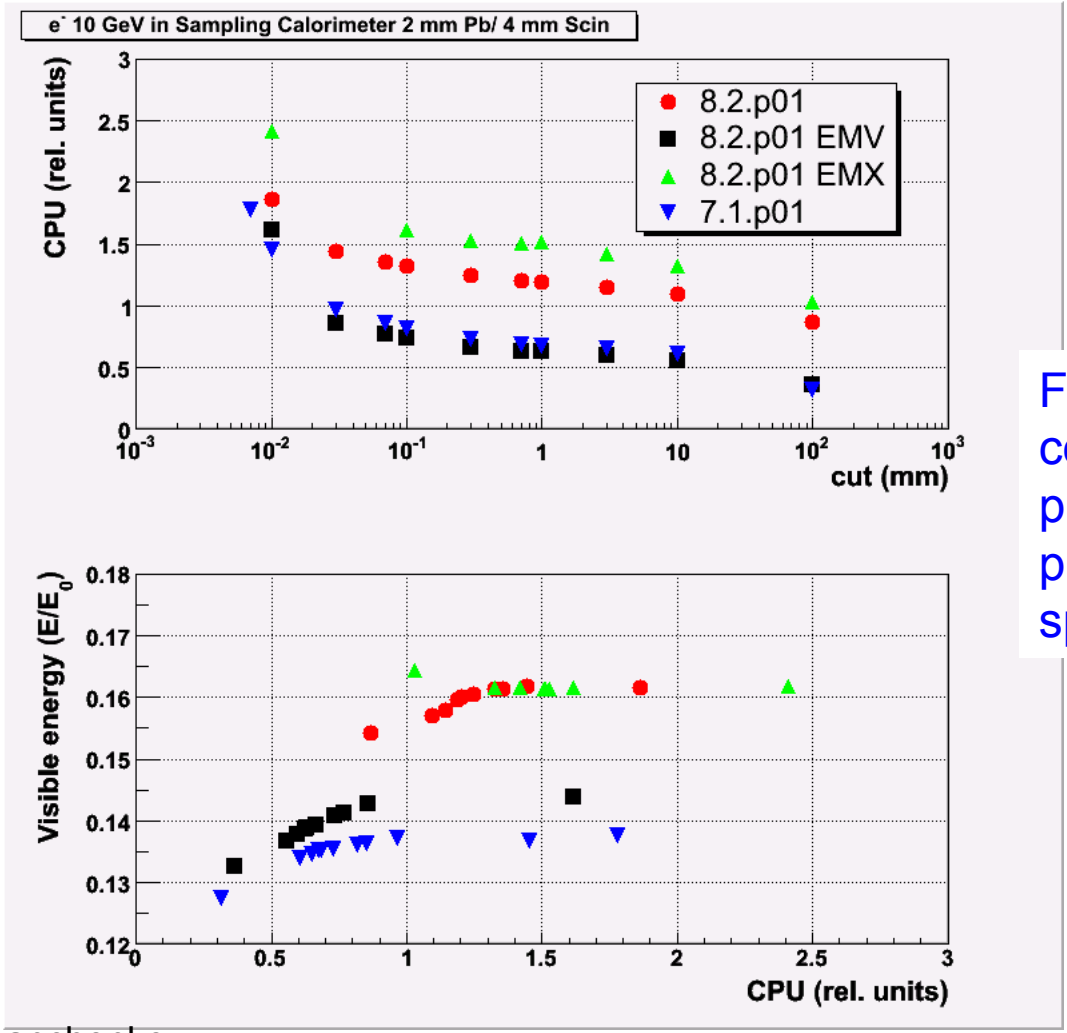
Estimates in LHC experiments computing TDRs based on past Data Challenges

Performance vs. Geant3

- **Application based on Geant4 compared to previous Geant3-based also in the term of performance**
  - **Observations varied from comparable values to substantially slower (up to 1 order of magnitude)**
    - **ATLAS, CMS, LHCb factors 1.5 – 2**
  - **Tuning of parameters**
  - **Tracking cuts on E_{kin} introduced in applications as special stepping actions**
    - **VCM/Alice, Gauss/LHCb**



Performance vs. range cuts



Find most reasonable compromise between precision of modeling physics processes and speed

from V. Ivanchenko

Choice of range cuts

- **Very different range cuts in the various experiments**

CMS

Beam pipe: 0.01 mm in Be, 10m elsewhere

Trackers: 0.01mm in pixel and 0.1m in trackers sensitive parts, 1mm in pixel dead regions, 5 mm in the TIB_Ledge, 10 cm elsewher

ECAL: 0.1m in Preshower sensitive, 1mm elsewhere

HCAL: 1mm for e's, 10mm for gamma's

Muon: from 0.002mm to 10 cm

ATLAS

LAr calorimeter: 0.03 mm

Muon drift tubes: 0.005 mm

Elsewhere: 1mm

LHCb

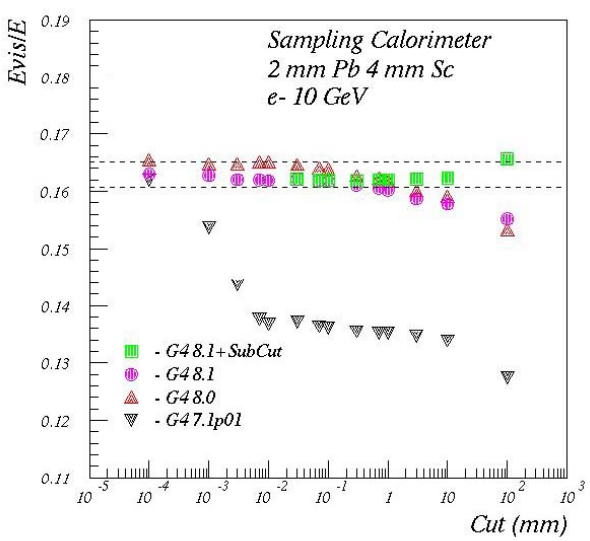
10 mm for gamma's

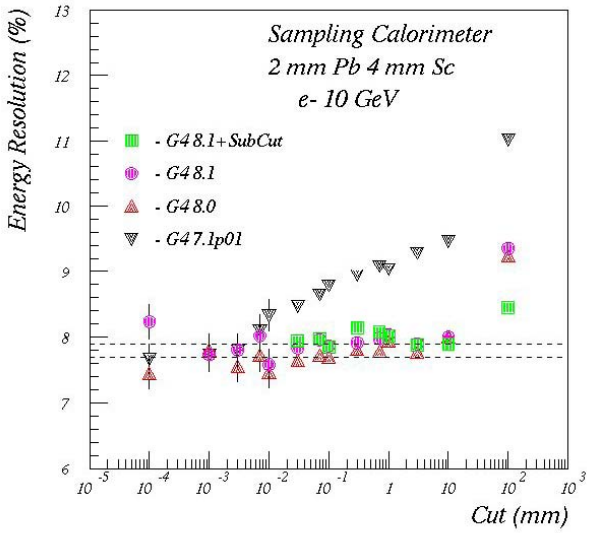
5 mm for e+

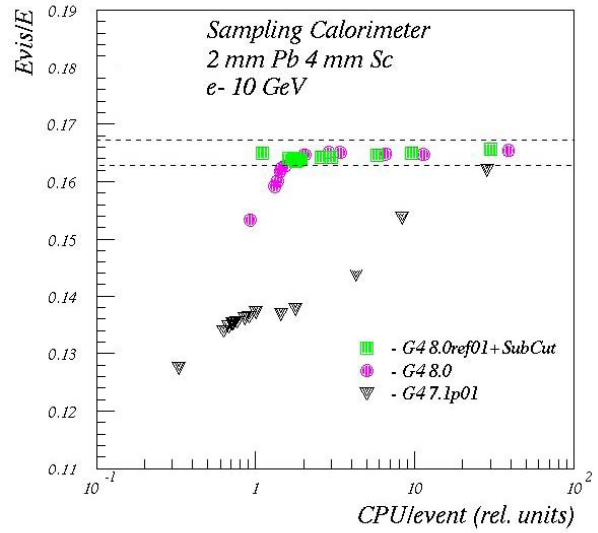
10 km for e- to have delta-rays off in trackers but affect dE/dx

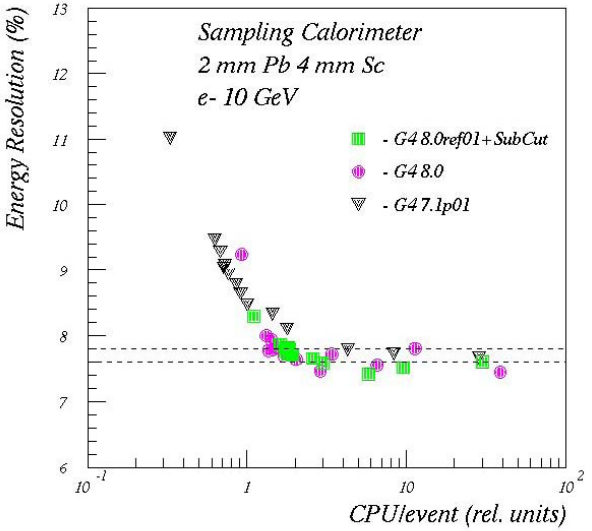
- **But also very different geometries between and in them.**
  - **Starting points not the same for thin 200 μm silicon and calorimeters**
  - **Depend also on how the digitization of a detector is done**

Performance vs. range cuts









Performance vs. Geant4 versions

- **ATLAS, CMS and LHCb experiments have done or are doing major productions with Geant4 7.1.p01.**
  - **ex. LHCb produced ~ 300 M events in data challenge DC06**
    ~ 28 s/ev min bias and ~ 86 s/ev for b @ 2.8 GHz

- **They are now concentrating their efforts in validating the latest of the Geant4 8 releases (8.2.p01)**
  - **Warning from Geant4 team of likely impact of major changes in EM standard physics introduced with Geant4 8.0**
  - **Several tests done by ATLAS/CMS in order to understand the impact on the experiments of the new Multiple scattering**
  - **Three variants of EM standard physics for LHC in 8.2.p01**

Performance vs. Geant4 versions and EM physics

ATLAS Results with full detector

Range cut 1 mm

With MSC from G47,1

Without step limitation

	G4 7.1.p01	G4 8.0.p01 - Ratio vs. 7.1.p01			
		Default	1mm	msc71	nsl
Susy	896.46	2.25	1.89		0.95
$Z \rightarrow ee$	890.47	2.15	1.77	0.96	0.85
$Z \rightarrow \mu\mu$	713.76	1.92	1.68	0.90	0.94
$Z \rightarrow \tau\tau$	750.73	1.90	1.67	0.99	0.90
$H \rightarrow llll$	862.15	2.07	1.66	1.03	0.91
Jets	685.8	2.10	1.99	1.02	1.10

CPU time per event [kSI2K]

Same simulation software (Athena release) built with different version of G4

~ 250 events per sample

G4 8.0.p01 with default physics list needs about twice the time of G4 7.1.p01

Similar time performance without step limitation and MSC 7.1

Performance vs. Geant4 versions and EM physics

ATLAS Results with full detector

Tuned for low CPU

EM to mimic G4 7.1

	G4 7.1.p01	G4 8.1.p01 - Ratio vs. 7.1.p01		
		QGSP	QGSP_EMX	QGSP_EMV
Susy	1000.06	1.94		1.55
$Z \rightarrow \mu\mu$	723.4	2.01	1.50	
$Z \rightarrow \tau\tau$	799.96	1.94	1.43	1.08
$H \rightarrow llll$	884.52	2.06	2.35	1.02
MB	284.59	2.02	1.48	1.14

CPU time per event [kSI2K]

G4 8.1.p01 QGSP similar to 8.0.p01

G4 8.2.p01/QGSP_EMV reproduces computing performance of G4 7.1.p01

	G4 8.2.p01	
	QGSP	QGSP_EMV
Susy	1706.6	992.36
$Z \rightarrow ee$	1643.07	962.83
$Z \rightarrow \mu\mu$	1372.53	806.53
$Z \rightarrow \tau\tau$	1322.46	802.98
$H \rightarrow llll$	1563.48	1122.81
Jets	1331.88	298.42
MB	493.98	935.51

Test done on different Athena builds than 8.1

Performance vs. Geant4 versions and EM physics

CMS Results with full detector

	G4 7.1.p01	G4 8.1.p01/Ratio vs 7.1	
		QGSP	QGSP_EMV
H → eeμμ	247.2	1.71	0.80
MB	47.59	1.30	0.78
Heavy Ions	5976	1.35	0.88

~ 50 events per MB and Higgs

~10 events per Heavy Ions

CPU time per event [sec on 3.6 GHz]

Same simulation software (CMSSW) built with different version of G4

Tests repeated with high statistic samples (10 k events) for 8.1.p02 and 8.2.p01

G4 8.2.p01/QGSP_EMV shows improved performance respect to of G4 7.1.p01

H → 4μ and single 1TeV μ ~ 10 -15 %

MB 20 – 25 % and Z' → dijets ~ 15 %

1 TeV e^- and π similar

With 8.2.p01/QGSP CPU speed degrades ~ 10 % for min bias and 15% for Z'. EM showers seem to improve vs. previous 8.1 series, ~ 35% instead of ~ 45 – 50%

Physics lists (a parenthesis)

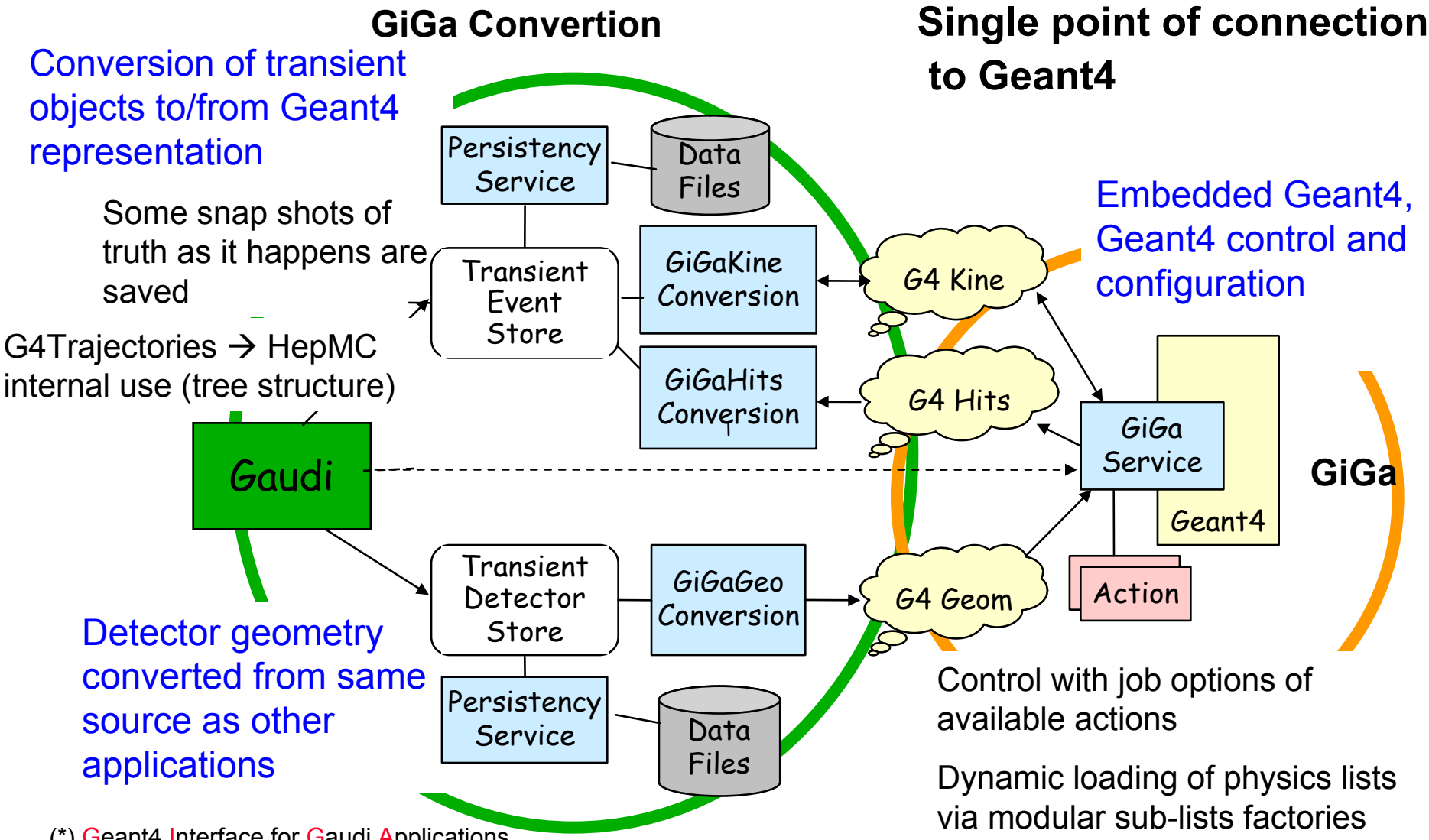
- **Physics lists are very useful**
  - Makes it easier to do tests/comparison
  - Many variants of hadronic physics for different regimes
  - For HEP mostly use QGSP, QGSC and LHEP
  - 3 variants of EM standard physics for LHC at the moment
- **Can be used as-is or as starting point**
  - Would be nice to have better documentation of what processes are for what energy range.
- **From 7.1.p01 to 8.2.p01 reference physics lists part of source**
  - Same builders used in G4 examples and tests
  - User and developer community have the same reference physics
- **HEP experiments are complex systems with very different components**
  - one detector background to another
  - optimize simulation of overall detector only with tuning of parameters otherwise very difficult to maintain and debug

Geant4 and experiments software

- **HEP experiments have their own software frameworks and use Geant4 in that context**
  - **Athena (ATLAS), CMSSW (CMS), Gauss (LHCb), VMC (ALICE, CBM@GSI, Minos)**

- **Experiment applications provide**
  - **Connection to event generators**
    - **consistency of decays**
  - **Event model for MC truth and Persistency**
    - **Access to snap-shots of process to understand**
  - **Histograms, messaging**
  - **Physicists in the experiments are shielded from Geant4 to different degrees**
    - **different in the various experiments**
    - **different for different roles**

Gauss and Geant4 (LHCb)



(*) Geant4 Interface for Gaudi Applications

Virtual Monte Carlo and Geant4 (ALICE)

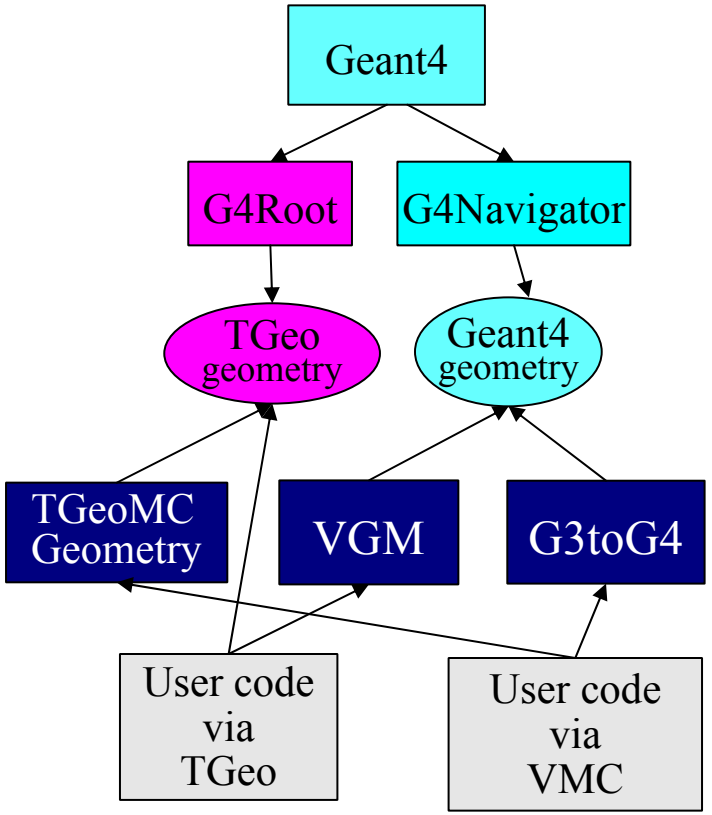
- **Makes user application independent of specific transport code**
  - **GEANT3, GEANT4 and FLUKA supported so far**
  - **Keeping the SAME definition for geometry, I/O formats and detector response simulation**
    - **Allows running the same application with different MC's**
  - **Provides MC-independent API for**
    - **Geometry definition (a la Geant3), setting up physics, setting up cuts, handling particle stack … (features very different from one MC to another)**
    - **Querying MC machine state and kinematics during stepping callbacks (very similar mechanisms)**
- **Provides several geometry converters**
  - **eg. VGM (G4 ↔ XML (AGDD, GDML) ↔ TGeo)**
- **Provides a multi-purpose geometry engine independent from any MC software, ROOT TGeo**
  - **Optimized for navigation performance in detectors geometries**
  - **Can be used as navigator for all transport MC's**

VCM and geometry

- **TG4RootNavigator specializes G4Navigator**
  - **Implements methods for locating a point, finding the distance to next boundary, computing the safety distance and the normal to a crossed surface**
  - **Very useful help from GEANT4 team in changing some methods/data members qualifications – made the implementation easier**
  - **Can be used with Geant4 8.2**

With geometry definition via both VMC and TGeo possibility to run with both G4 native and G4Root navigation

- **Geant4 VMC connects automatically necessary packages and activates selected navigator**



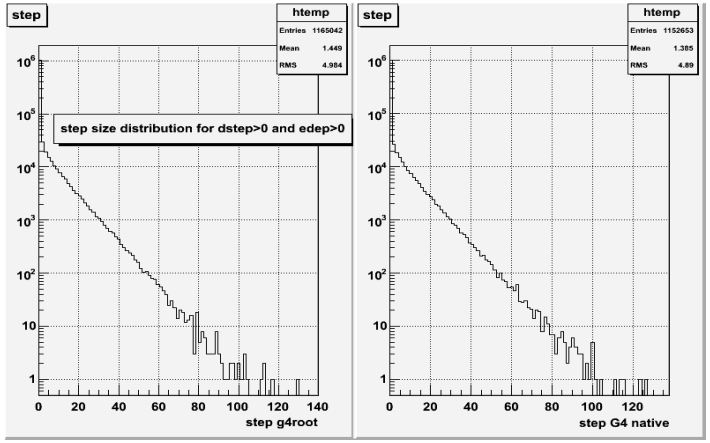
Most example (N01, N03, N05, N06) give identical results

Performance vs. Navigator

ALICE Results

Performance comparison require complex geometry

AliRoot – offline framework using GEANT4_VMC for simulation



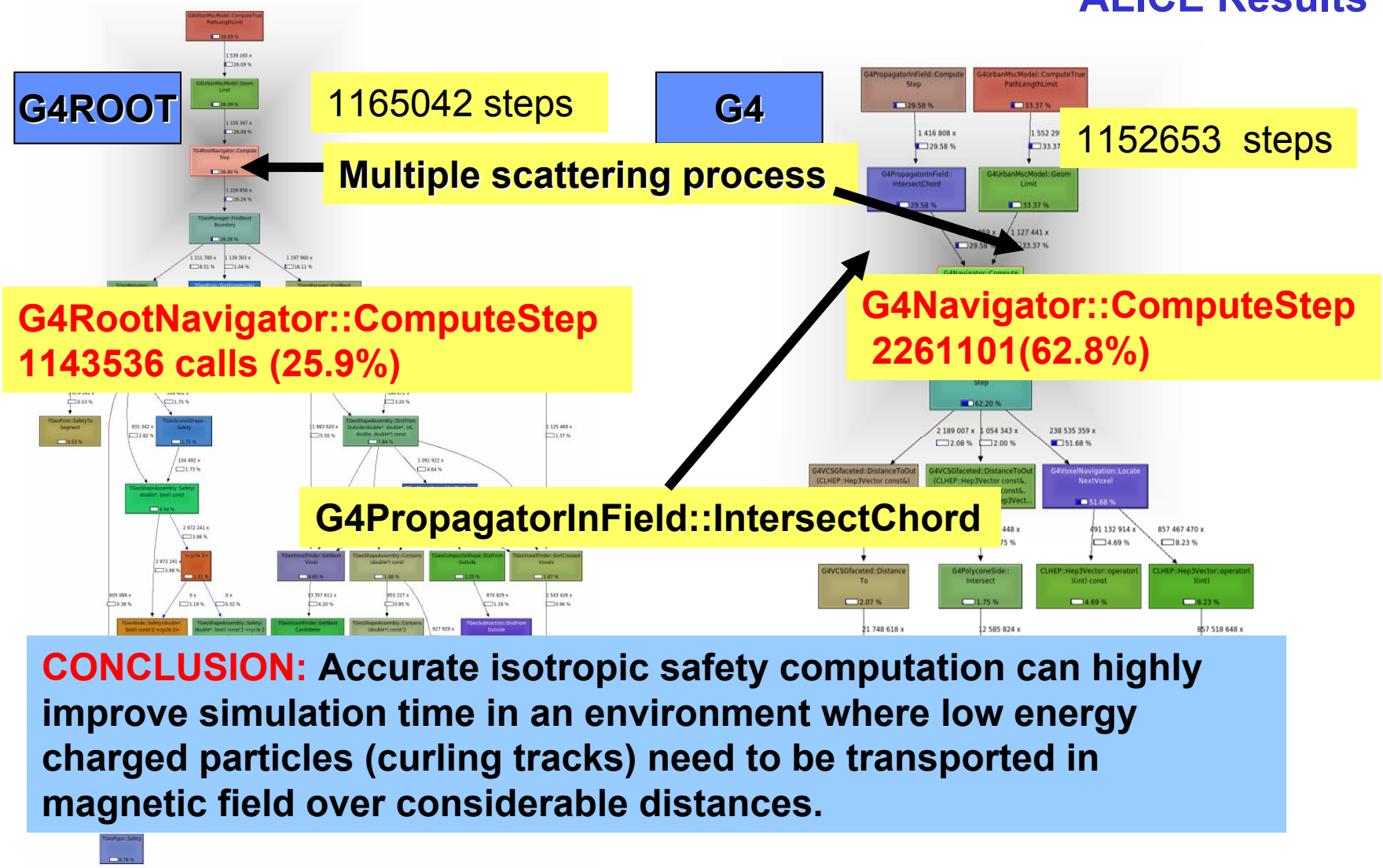
Step length distributions are identical

	TGeo	G4Navigator
100K geantinos TPC	200 sec	225 sec
5K particle, physics (0.5-999 GeV) + field	1013 sec	2144 sec
10K geantions muon arm	27 sec	26.4 sec

TGeo navigator ~ 2x faster with magnetic field and physics particles

Performance vs. Navigator – Profiling

ALICE Results



CONCLUSION: Accurate isotropic safety computation can highly improve simulation time in an environment where low energy charged particles (curling tracks) need to be transported in magnetic field over considerable distances.

Performance vs. machine architectures

ATLAS study with 3 configurations

- 32/32 = 32bit build on 32bit machine
- 32/64 = 32bit build on 64bit machine
- 64/64 = 64bit build on 64bit machine

	Ratio of kSI2K wrt 32/32	
channel	32/64	64/64
susy	1.28	1.18
Zee		
Ztautau	1.26	1.16
H4l	1.32	1.12
MB	1.28	1.2
jets	1.07	0.94

	Ratio of seconds wrt 32/32	
channel	32/64	64/64
susy	0.72	0.66
Zee		
Ztautau	0.7	0.65
H4l	0.72	0.61
MB	0.69	0.66
jets	0.56	0.49

Normalized to kSI2K using conversions factor provided by LSF. May not be 100% accurate to compare 64bit and 32bit architectures.

Only dbg build available when doing measurements

Robustness

Crashes and aborted events impact mass production

High rate implies loss in amount of events and resources

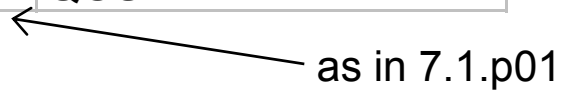
When producing millions of events small problems come to light

Also for robustness check need complex geometries

Global robustness

- **CMS reported a high number of crashing jobs for Minimum Bias and Z' → dijets events with G4 8.1.p02 and QGSP**
  - **crashes tracked down to stuck tracked and incorrect handling of G4ExceptionHandler when an event was aborted in the CMS application**
- **ATLAS reported ~ 76% of events of physics aborted (stuck tracks) with G4 8.2.0 out-of-the-box and QGSP**
  - **~ 5% with G4 8.1**
- **Close collaboration with G4 developers to fix the problem**
  - **Combination of MSC intensive use of Navigator and overlaps**
  - **With G4 8.2.p01 ATLAS observed ~ 10% aborted events**
  - **LHCb observed**

~ 6 - 7 %	QGSP/LHEP
~ 6 - 7 %	QGSP/LHEP + EMX
~ 0.5 %	QGSP/LHEP + EMV



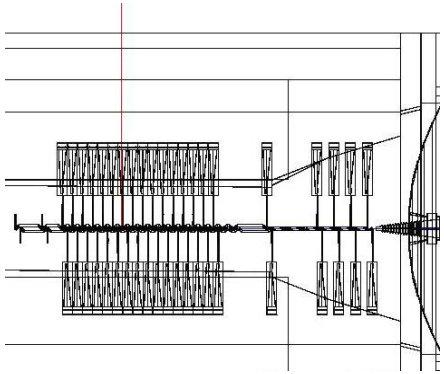
  - **ATLAS tested development tag and it seems to completely solve the problem**

Global robustness

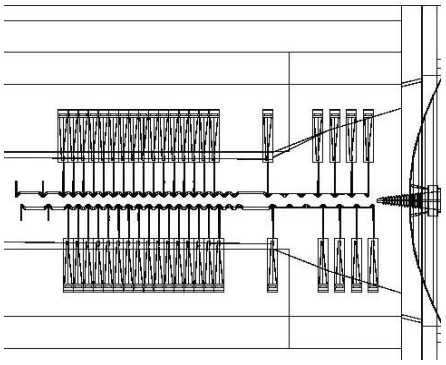
- **CMS observed G4 7.1-based simulation went into infinite loop on NaN**
  - **Min bias : 0 – 2 events out of 1000**
  - **QCD : ~ 2 % of events**
  - **Heavy Ions : ~ 65% of events**
- **Tracked to numerical instabilities in G4 code fixed in G4 8.1**
  - **unprotected sqrt(a – b) in hadronic physics**
- **Tests of Geant4 8.1/8.2-based released show significant improvement performance**
  - **No NaN in 75 Heavy Ions events**
  - **Only 2 NaN in production-type tests (min bias few 10K events)**

Debugging problems

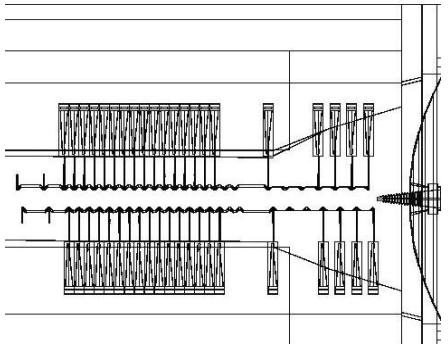
- **Many problems have been tracked to geometry and overlaps**
  - **Essential for new experiments**
  - **Even now LHC detectors are not frozen, pb. of misaligned geometries**



LHCb **Close Velo**



Semi Open Velo



Open Velo

  - **Useful to have tools to check overlapping tools and to debug geometry**
  - **Improved visualization**
    - **cut away ¼ or ½ detector to show innards (also with events shown)**
    - **visualization of boolean solids**

Debugging problems

- **Important to trace back reason of crashes**
  - **Detailed information available in hadronic phyisics when a problem occurs for foreseen reason is present and very useful**

```
G4HadronElastic WARNING ekin= -1.1368684e-13 after scattering of neutron
p(GeV/c)= 8.7697033e-05 on proton
In src/G4ReactionDynamics.cc, line 3877:
===> G4ReactionDynamics::NuclearReaction: inelastic reaction
kinematically not possible
  G4HadronicProcess failed in ApplyYourself call for
  - Particle energy[GeV] = 2.2737368e-16
  - Material = LiquidArgon
  - Particle type = neutron
```

- **Detailed printout for normal situation**
  - **very important when developing or adopting a new Geant4 version**
  - **can clutter log files and should be under the control of the user: improved in recent release.**

Releases

Experiments need stable applications for mass production

Cannot change physics content within a "defined" production

On the other hand would like fast technical patches

Bug fixes for crashes and memory leaks
Time improvements if transparent

Releases

- **Time delay for experiments to adopt a new Geant4 release (in production)**
  - **The (HEP) experiments frameworks or applications that make use of Geant4 may need to be adapted to new version**
    - **ALICE VMC, ATLAS Athena, CMS CMSSW, LHCb Gauss, …**
  - **Small tests allows to find big problems**
    - **With Geant4 8.2 70% of the events stuck in ATLAS**
    - **Impossible to run a given physics list for CMS**
  - **Production-type tests necessary to find more subtle/rare problems and for physics and performance validation**
  - **More rare problems are found once operational**
  - **Deploy the use of a G4 release in production**
    - **At the moment for LHC experiments impact on Data Challenge if major problem (delay or keep previously deployed release)**

Releases

- **Finding problems as early as possible eases and speeds up the process**
- **Once experiments will have data will want to do it as fast and with as little impact (but the wanted one!) as possible**
  - **Untested features can generate possible unpredictable delays in the whole chain**
- **Useful to discuss new major features and impact (when known) in detail**
  - **List of tasks are presented at G4 Technical Forum**
  - **Selected topics are presented at Physics validation meeting**
  - **Decide to adopt a given release**

Releases

- **Appreciated advanced warning about CPU increase of EM physics in Geant4 8.0 given at Technical Forum**
  - **even if not happy about the content of warning**
- **In release note it would be useful to have the higher level reasons for the changes in addition to the specifics. It would help to understand the impact and better judge if/when to adopt the release.**
  - **"Fixed problem for low energy hadrons" is not clear. What was the problem? What does it mean low energy here? In which type of applications there will be an effect?**
- **Would help to have references to results of tests performed before a release**

Releases

- **Necessary to find the problems as soon as possible**
  - **Complex geometries necessary to evaluate both reliability and performance**
  - **Some LHC experiments (could) have the possibility of saving their geometry in GDML**

- **Useful to have patches available before release to test**
  - **ex. ATLAS tested development tag to investigate abort rate observed in 8.2.p01**
  - **Spot problems before releases, although sometimes time conflict**

Summary

- **Time performance a big concern**
  - New multiple scattering treatment improves the data/MC description but big increase in CPU
  - User control of physics quality vs. statistic needed
- **Reliability improved from first versions used in production but recently major problems in G4 8.2**
  - Seems to be solved with latest development
  - Many problems related to geometry both for overlaps and in code
- **Easier to use than at the beginning**
  - Physics list very useful
  - Documentation, tutorials on the web very much appreciated
- **Avoid surprises**
  - Communicate reason and impact of new features
    - Time performance
    - Variation of visible energy
- **Long process to adopt new G4 releases, try to minimize it finding problems early**