Updates
on requirements
from previous TF meetings

Geant4 Technical Forum
December 1st, 2005

John Apostolakis (CERN)
on behalf of Geant4 collaboration

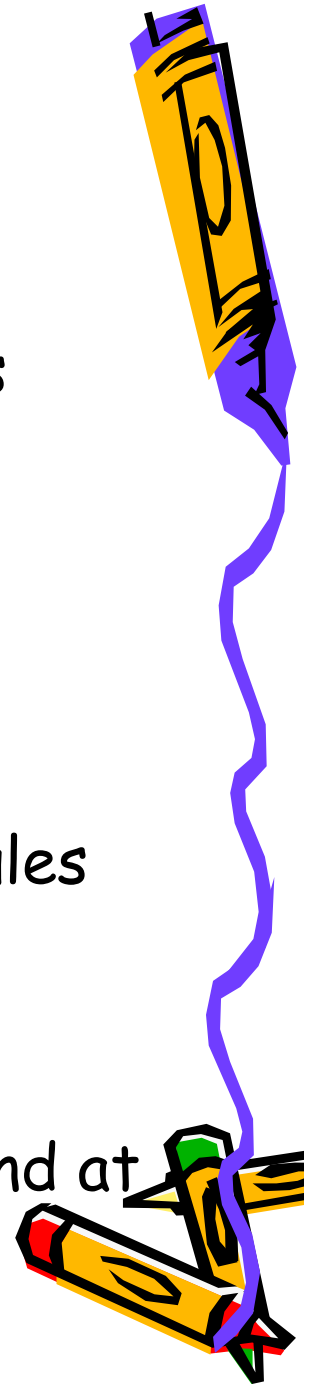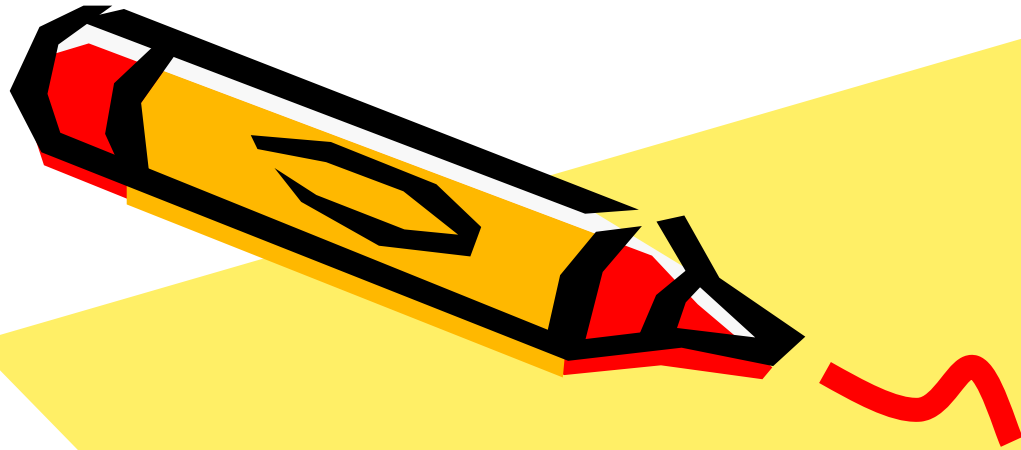δs

Outline and links

Outline

- Update on requirements for which the status has recently changed
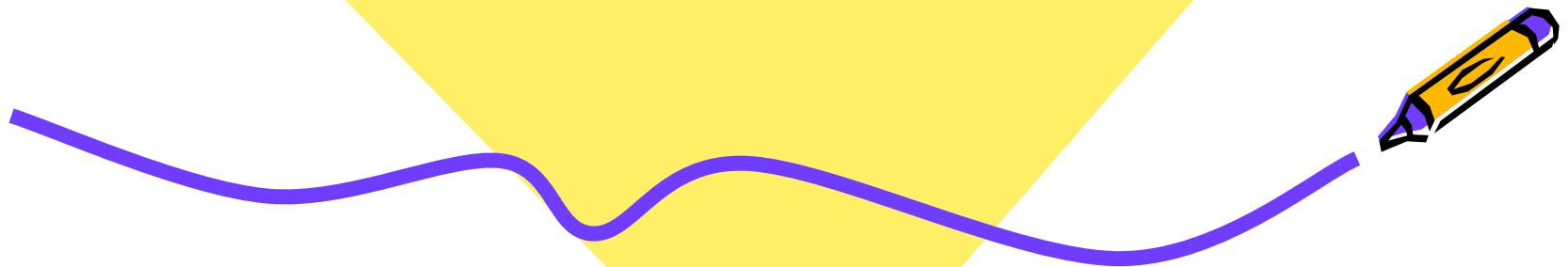- Open requirements
- Long-term requirements

Some links

- Updated work plans and expected release schedules can be found at

  http://cern.ch/geant4/source/planned_features.html

- Previous updates at Technical Forums can be found at
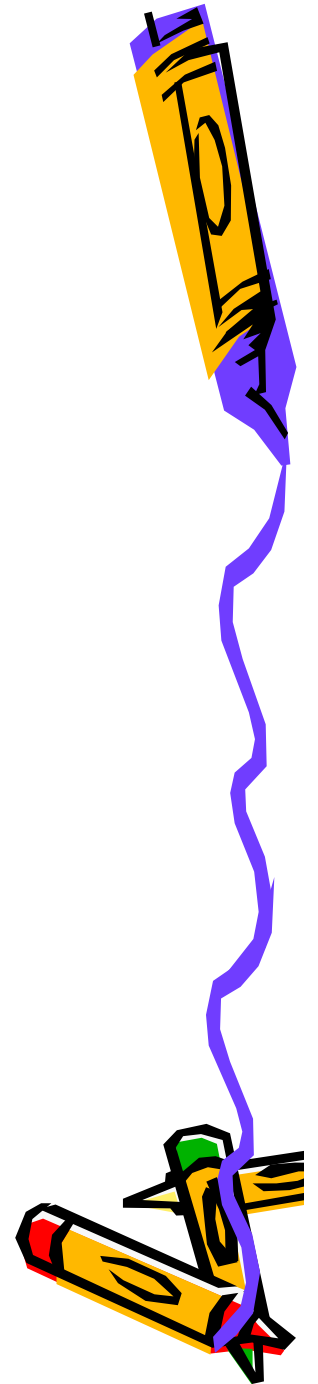
  http://cern.ch/geant4/technical_forum/

Recently closed or suspended

Requirements closed by G4 v7.1

- Req. 0701: Polarised Rayleigh scattering
- Req.0705: User Limits per region

701. Polarised Rayleigh scattering

Originator: PoGO (Tsunefumi Mizuno)

Responsible : M.G. Pia

- Need Rayleigh scattering process that includes photon polarization, as neglecting it gives an artificially small modulation.

  - Rayleigh scattering cross section is not negligible in the energy of our interest, this needs to be solved to simulate accurately.

- Request to implement the polarization process in Rayleigh Scattering

Status

  - A LowEnergy Polarised Rayleigh process was released in Geant4 7.1 (June 2005).

  - Feedback from users would be appreciated.
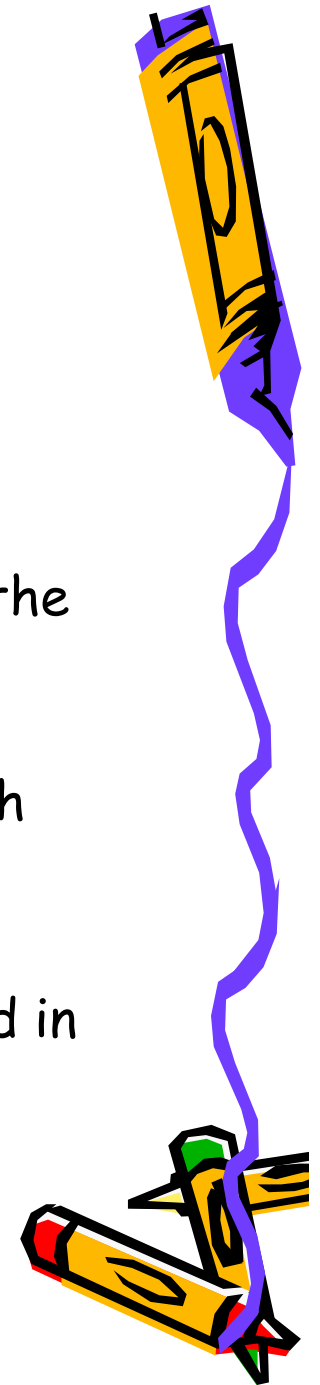
705. User Limits per region
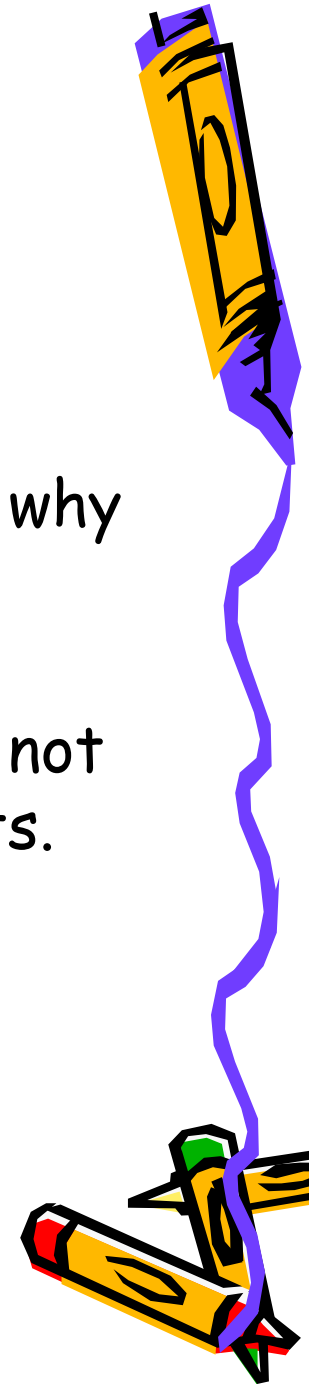
Originator: EXO experiment (SLAC)

Responsible: M. Asai

- Enable choice of User Limits per region

- "Given Geant4 allows defining cuts per region, why it does not allow defining G4UserLimits to a region?"

Notes: A first examination showed that this will not conflict with existing use cases for User Limits.

Status

- Delivered with 7.1.

- To be closed.

Originator : Atlas/CMS
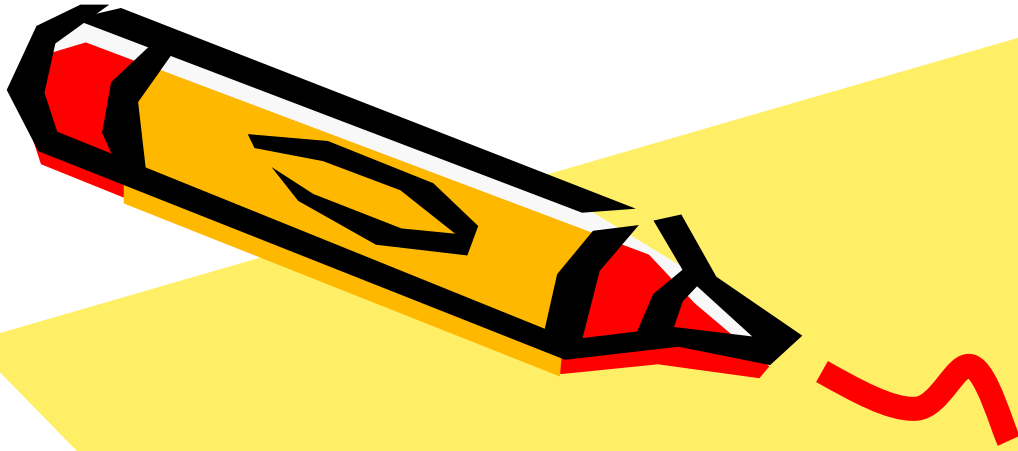
Responsible: J. Apostolakis, M. Asai

Example for creating new type of particles: creating a new particle and a modified primary transformer that creates tracks
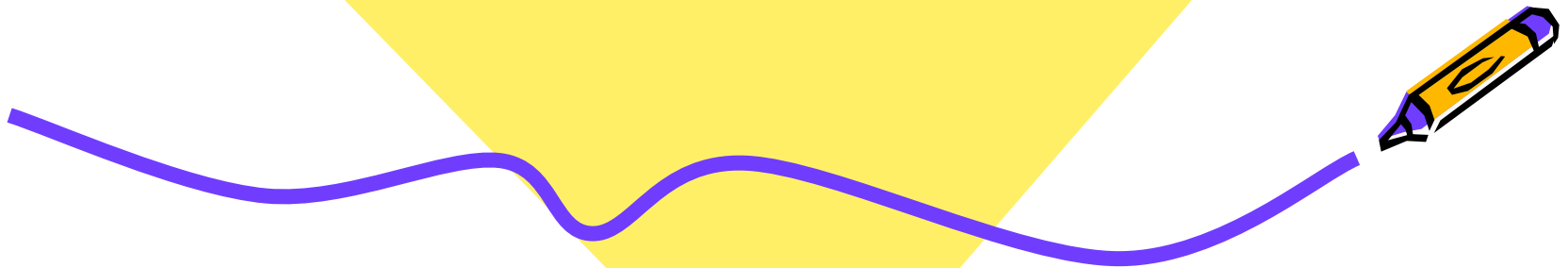
Use case: creating new heavy sleptons particles, to investigate potential new physics in LHC experiment detectors.

- Requestors have their own working codes. Thus they do not still request this.

- Suspended

Latest updates

Req.0313: Particle properties from an external source

Responsible: M. Asai, H. Kurashige

Requestor: LHC

Description: "Request to study whether one can have a unique definition of the particle properties throughout all the physics models within G4 and preferably also consistent with the values used in generators. A candidate catalogue can be HepPDT, extracted from the PDG tables."

- Design study, implementation, performance tests, and assessment of effects on user code achieved 1H2005.
  - Refinements and resulting changes in G4 source, 2H2005.
- Latest (Nov 2005)
  - Developments scheduled for inclusion in Geant4 ver 8.0.
    - "non-static" particle definition
    - revised hadronics physics lists.
- Restriction: Use for resonances is not foreseen now – would need studying
  - some physics models require particular values of mass/width for particular resonances (in general poorly measured).
- Note: gcc 2.95.X is not supported.
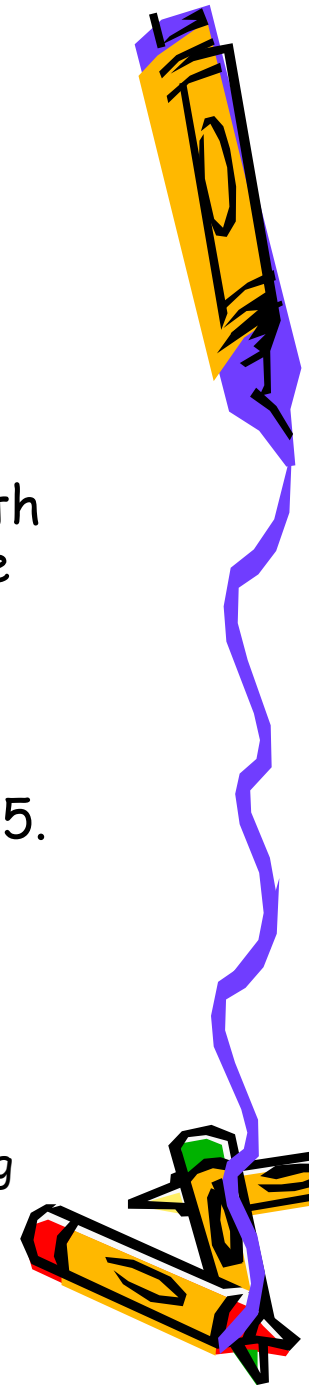
Req 0313: Impact / considerations

The capability is now enabled to change particle properties. There are caveats, though, regarding for which particles such changes can be made, and what changes are possible without impacting Geant4 results.

A first assessment

- For heavy particles, like B, C, T meson/baryon and W/Z bosons, there are no physics in Geant4, and so no impact.

- For light leptons (e, μ), there is a conflict if masses are modified.

- For mesons/baryons
  - some changes are safe for light stable particles
  - Properties of resonance must be maintained.

- In general, the impact of changing of particle properties depends on user requirements and use cases and will require in-depth information on these in order to assess fully.
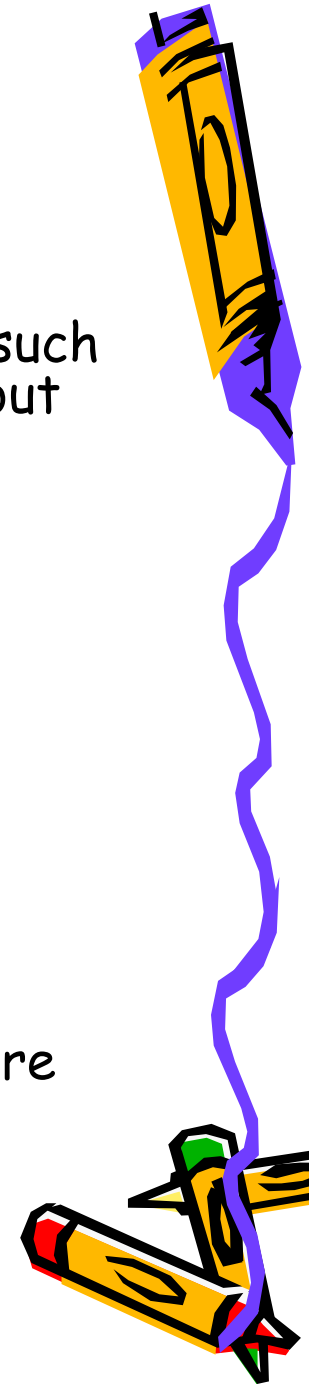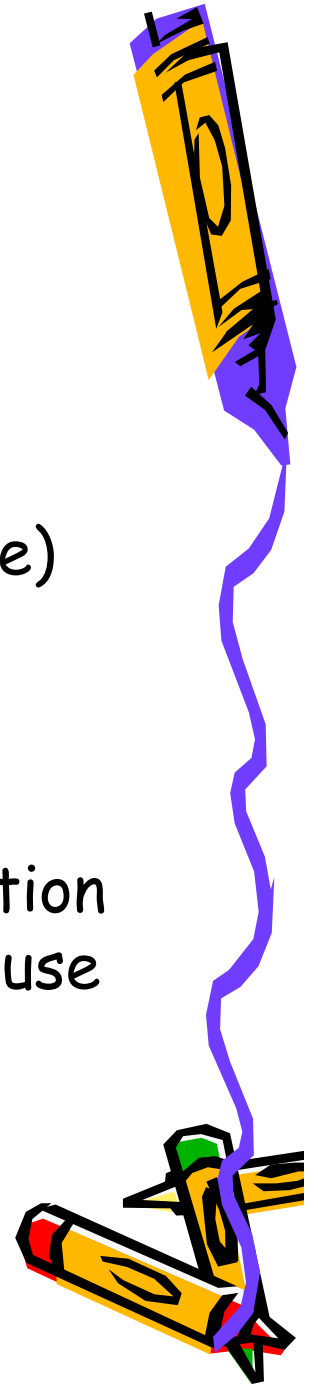
Req.0403: Unique set of physics lists

Responsibles: V. Ivantchenko / G. Folger / M.G. Pia

Requestor: ESA (G. Santin)

Description: "Unique set of physics lists (by use-case) and not two sets as now, one for EM and one for hadronics."

Latest

Physics lists (for hadronic use cases) under preparation and scheduled for inclusion in release Geant4 8.0 use the EM physics builder from EM(std).

Req.0501: Print-out of created processes should be optional

Responsible: M. Maire / M.G. Pia

Requestor: LHCb, Atlas

Description: "The list of created processes is printed out at the beginning. Though it is useful for development and verification, it should be possible to switch-off for mass production run."

Status:

- Option in EM(std), verbose level -1 stops print-out.
- LHCb reported difficulties in utilising this
  - reason now identified (no 'PreInit' actions in LHCb)
- Could study also potential driving from physics list

Req.0502: Treatment of particles that get stuck during simulation

Responsible: G. Cosmo, J. Apostolakis

Requestor: CMS, LHCb

Description: "CMS drops a track if it is stuck and continues the event. G4 by default abandons the event. Neither is good."

Status

- In Geant4 7.0 a stuck track is given additional kicks and chances to continue
    - only most problematic 'stuck' track is killed.
- To make additional effort to keep high energy particles (> 500 MeV)
    - See further discussion on Req.602.

# Req.0602: Protect high energy particles from loop killing

Originator: CMS: (P. Arce) Old title: Tracks killed by G4Transportation

Responsible: J. Apostolakis

- G4Transportation kills a particle if during an step in magnetic field it has looped more than 1000 times without finding the boundary:
  - In CMS min-bias events in CMS saw this **68.1 times per event**
    - Average energy lost is ~1 GeV / event
- Some tracks have E > 1 GeV (in 7K events highest was 13.7 GeV)

Updated status:

- Protection avoiding to kill particles above 100 MeV (unless stuck 10 times) added to Geant4 7.0
  - CMS now sees ~1.5 tracks killed per min-bias event (7.1p01, Nov05),
    - When using cuts for particles at around 100 MeV < E < 250 MeV
    - Report also seeing same number with G4 6.2 for these conditions.
- Resolution of underlying issues needs further joint study.
  - What are the key characteristic of killed tracks?
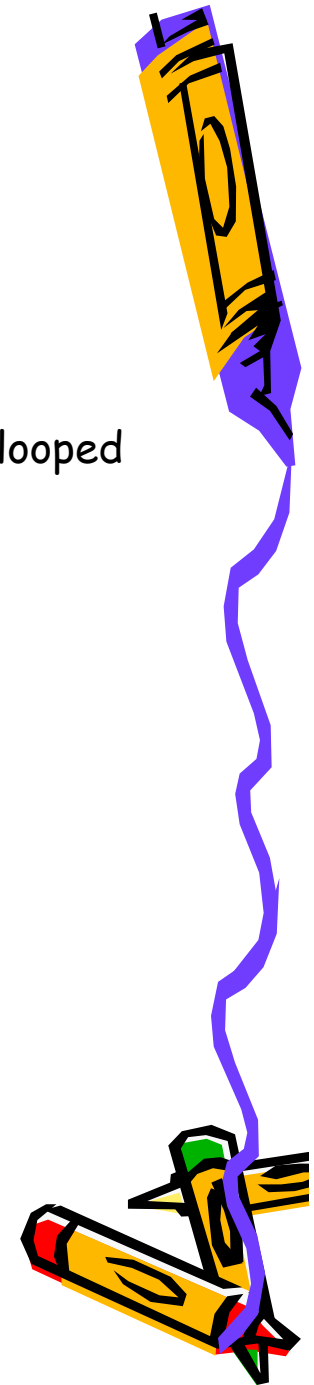
Req.0604: Nested parameterizations

Originator: M. Asai (on behalf of medical users)

Responsible: J. Apostolakis

Access to a touchable from "Compute" methods in G4VPVParameterisation class

 - Position, material, etc., could be parameterized with copy numbers of parent volumes (mother/ancestor) in addition to its own.

Status:

First version is scheduled for G4 release 8.0

- Interface enables use of 'parent' touchable providing access to full volume tree information

- Parameterization must specify materials (new methods)
    - Fix will be required to account for these material in region scanning

Restrictions:

- Only material, sensitivity and vis-attributes can be parameterized using information from parent(s)

- Dimensions, position & shape (solid type) must be depend only on its own copy number. Else cannot voxelize the logical volumes.

Req.0603: Option not to suspend tracks

Requirement from BaBar (D. Wright)

Responsibles (new) : D.Wright /A. Heikkinen (hadronics)

- Currently few processes which suspend particles.

- For BaBar applications, it would be very useful not to suspend the particle (at least in the hadronic processes).

- Details:
  - Processes involved are G4Cerenkov, G4Scintillation, G4FastSimulationManagerProcess, G4HadronicProcess
    - For G4HadronicProcess, only one hadronic model (G4NeutronHPElastic) invokes the suspension.

Discussion: An option adding a switch to a suspending process that enables the user to turn off/on the suspension of the particle could be a solution.
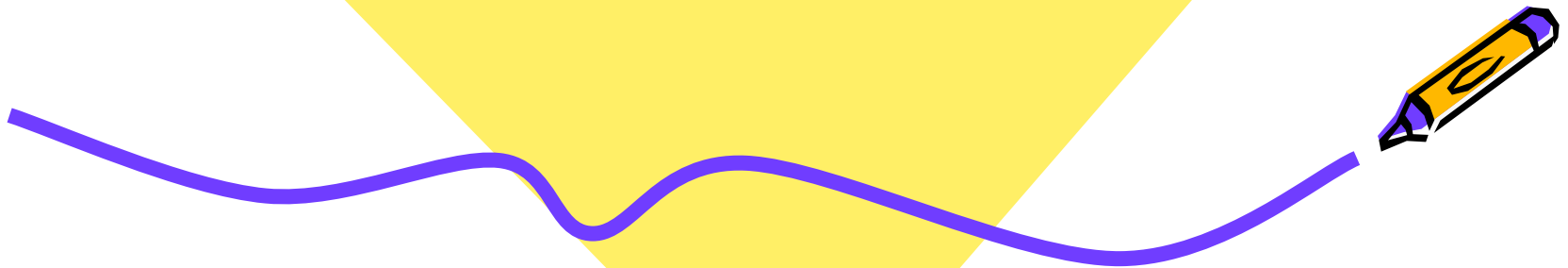
Status:

- G4Cerenkov, G4Scintillation and FastSimulation had such switches already.
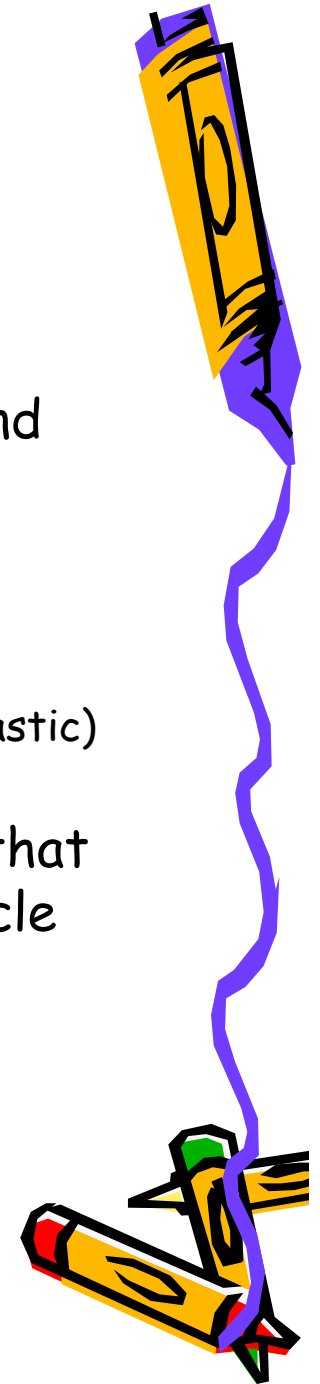
Other open requirements

Req.0505: Improvements in hadronics

Responsible (new): D.Wright /A. Heikkinen (hadronics)
Requestor: HARP

Description: "HARP needs following improvements in the energy
  range of 1-15 GeV."

- Bertini Cascade robustness for production - OK
- Binary Cascade extension to pion incidents – Done to 1.5 GeV
- CHIPS be available as alternative
- QGS model improvement to provide a smooth inclusive theta
  distribution in forward direction < 1 degree

Status

- G4 6.2 patch 2 included fix for a Bertini problem.
- Pion projectiles for Binary Cascade enabled in 6.0
  - Approach limited up to 1.5 GeV due to resonance data
- Improvements to QGS model theta distributions in forward
  direction (< 1 degree) underway.

Propose to close this 'multi-request/requirement' and open single-
  issue requirement for different parts.

Req.0601: More details in error messages

Responsible: J. Apostolakis, M. Asai, G. Cosmo
Requestor: LHCb (G. Corti), seconded by CMS

- To help in debugging problems in the production environment we wish to have detailed message when there is a problem. This already occurs for the hadronic physics and we have found it very useful. It would nice to have similar detailed message from the other parts of Geant4.

Information:

Typical message from G4HadronicProcess is

"Unrecoverable error for:
   - Particle energy[GeV] = 2.452
   - Material = Aluminium ;
   - Particle type = proton
 EXCEPTION: Fatal Exception number 007 in G4HadronicProcess:
    GeneralPostStepDoIt() failed on element selection."

This enables easy reporting of problem, and enables developers to find it. It makes it simpler to identify the cause, and therefore faster to resolve it.

Yet the conditions that allow this in hadronics (few calls and thus small overhead in terms of CPU time) do not exist in other key components: geometry and EM physics.

Discussion: What key areas and types of additional information are of most interest ? How much of performance overhead is acceptable ?
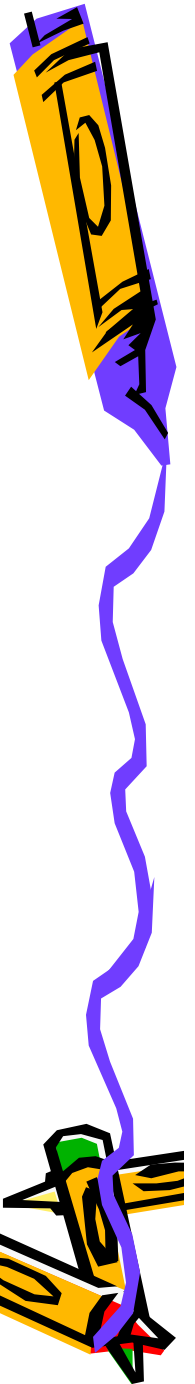
Req.0605: Adding touchable to secondaries

Responsibles: T. Sasaki and (new) D. Wright, A. Heikkinen, P. Gumplinger

- Touchable should be always attached for all secondaries
  - As of Geant4 6.2, only EM processes set it.

Status
- At 7.0, hadronic processes also add a touchable handle to secondaries.
- New (Dec 2005): Checking other processes has identified a few which do not assign a touchable (in case of position in current volume).
  - Found without touchable:
    - G4OpWLS (Optical process for wavelength shifting)
    - G4Cerenkov, G4Scintillation
    - Further study XrayTR radiation (issue regarding active volume)
  - OK were decay processes

- Note: Potentially can relieve individual physics processes, by doing it in kernel for secondaries created at step's end-position.
  - Issue for secondaries created at boundaries
  - Under consideration.
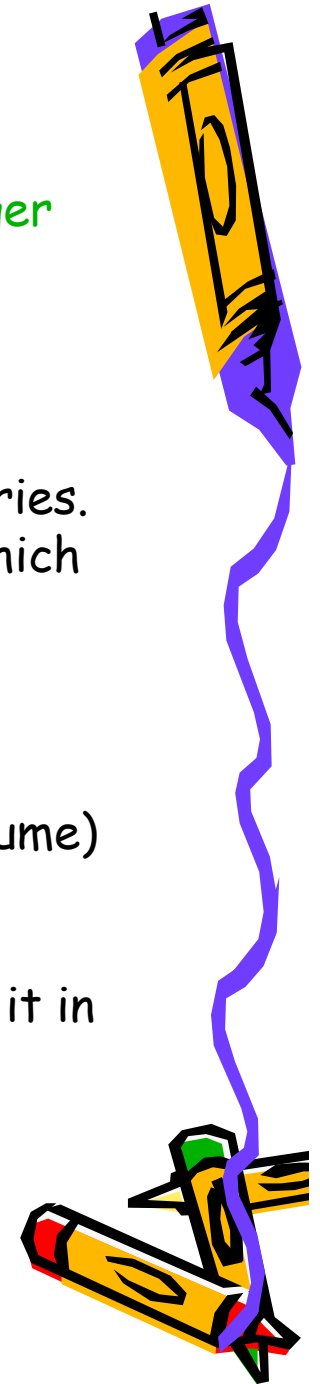
703. Treat particles with dipole moments

Originator: AD (Bertalan Juhasz)

Responsible: J. Apostolakis, H. Kurashige

- The user should be able to calculate the force acting on the magnetic (and possibly electric) dipole moment of a (neutral or charged) particle in an inhomogeneous magnetic (electric) field [F = mu * grad B]
  - for this, the magnetic dipole moment of a particle should be available for the equation of motion;
- Note: the magnetic moment is not always a vector of constant magnitude,
  - In magnitude and direction it can depend on e.g. the external magnetic field
- It should be possible to calculate the force by a user-derived equation of motion class

Comments/Status

- A first working solution has been identified – was communicated (Sep)
  - using existing classes and a few user derived classes
- For a solution 'integrated' in the toolkit
  - first design study done; prototype implementation to start.
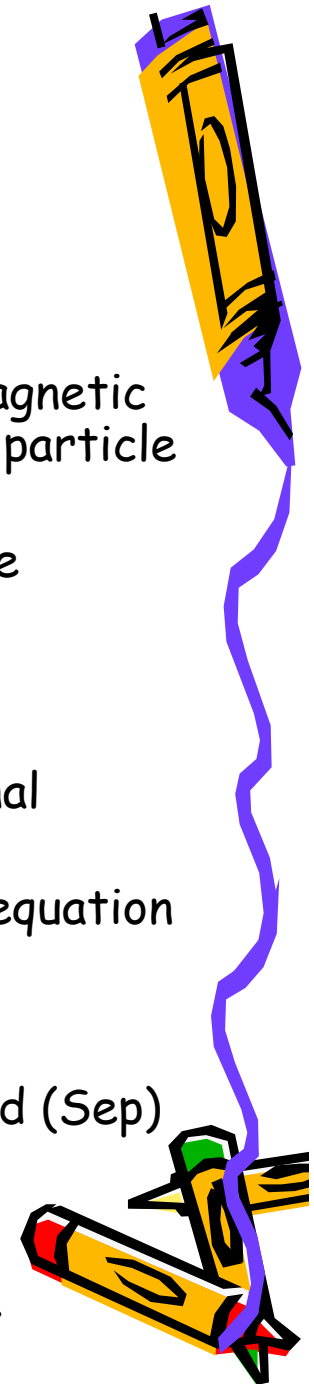
704. Neutron data for additional elements

Originators: (BaBar, Vanderbilt)

Responsible: D. Wright

- BaBar needs the elements Nd (Neodymium) and Sm (Samarium) added to the high precision neutron models.

- In addition Vanderbilt are asking that As, In, Ge, Ga, Sb, Hg, Cd, Te, and Gd also be added.

Seconded by ESA.

Status

- Most elements exist.

- Additional element (Hg) will be prepared.

707. Python UI

Originator : ATLAS (A. Dell'Acqua, A. Nairz)
Responsible: H. Yoshida

- More support for a python UI in G4 (not only the current UI/macro version).

- Plans for a 'broad-access' Python interface to Geant4 classes and their public methods were discussed at G4 Workshop (Bordeaux, Nov 7-10).

- Prototype developed, and refinements are underway preparing development release in 2006.
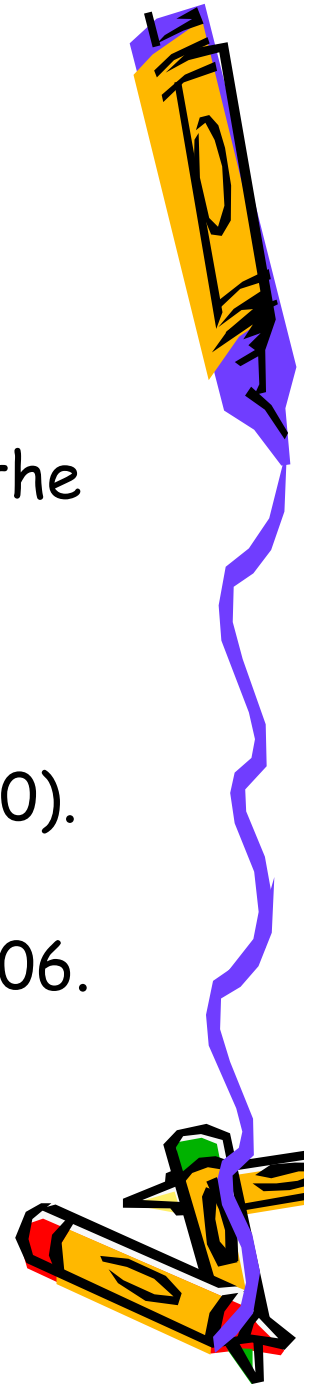
New proposed 'platforms': gcc 3.4.3

## Originator: ATLAS (D. Quarrie, A. Nairz)

Time: March 2005

- ATLAS, and the other LCH experiments, intend for the next two supported platforms to be:
  - gcc 3.4.3 with SLC3 in 32-bit mode (IA32)
  - gcc 3.4.3 with SLC3 in 64-bit mode (AMD64)
- Current understanding (to be checked) is that these are binary compatible with both Intel & AMD 32-platforms and EM64T Intel 64-bit platforms (not IA64 - Itanium).
- The [requested] timescale is that porting of external software to IA32 is about to start [3/2005] and we hope to have a prototype ATLAS port available in Sept 2005, but not yet in production.
- Also interested to maintain compatibility with CLHEP 1.8 for approximately the next 3 months.
- To be discussed separately.
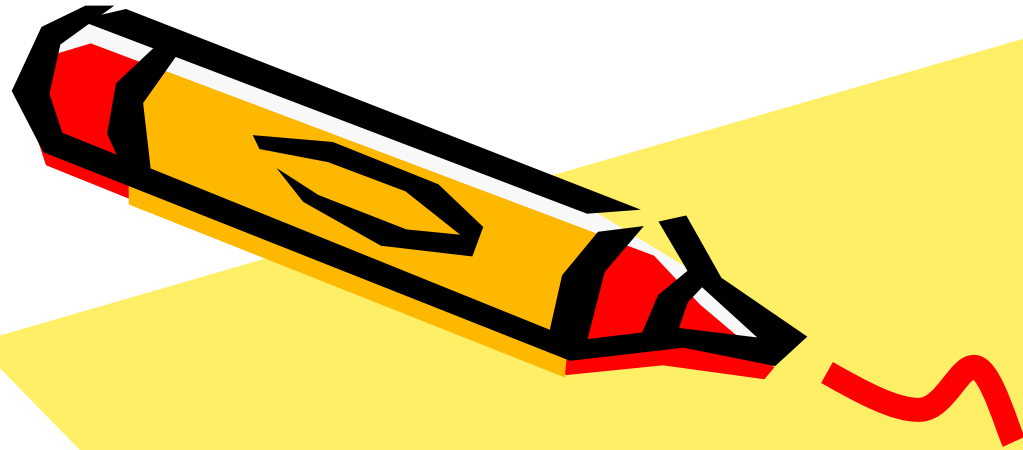
Longer term requirements
- Under development
- Under study
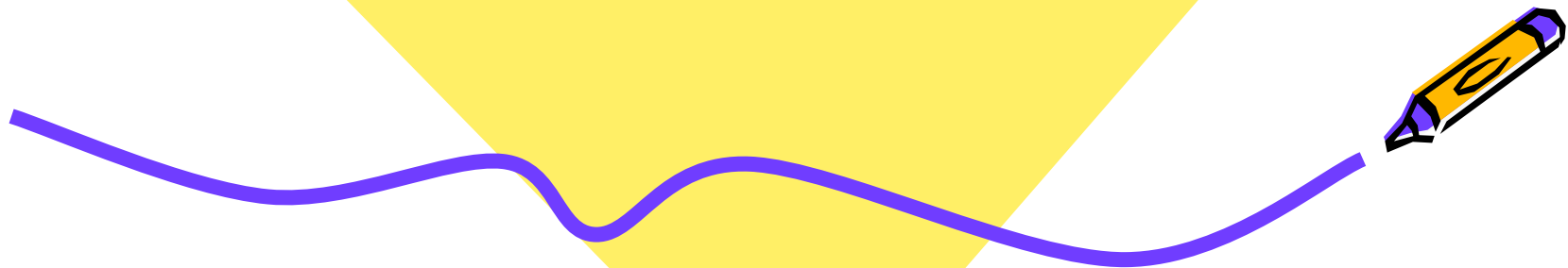
Req.0103 part 2: Geometry construction - input from external models

Responsible: G. Cosmo

Additional ways to input the description of the geometry of a setup via GDML and CAD-input.

Two aspects were identified:

- GDML moved to Req.0304 and closed
- CAD interface:
  - in the process of identifying objectives for
    - BREPs extensions and interface to CAD
    - We are discussing with NASA/GSFC and ESA for taking care of this.
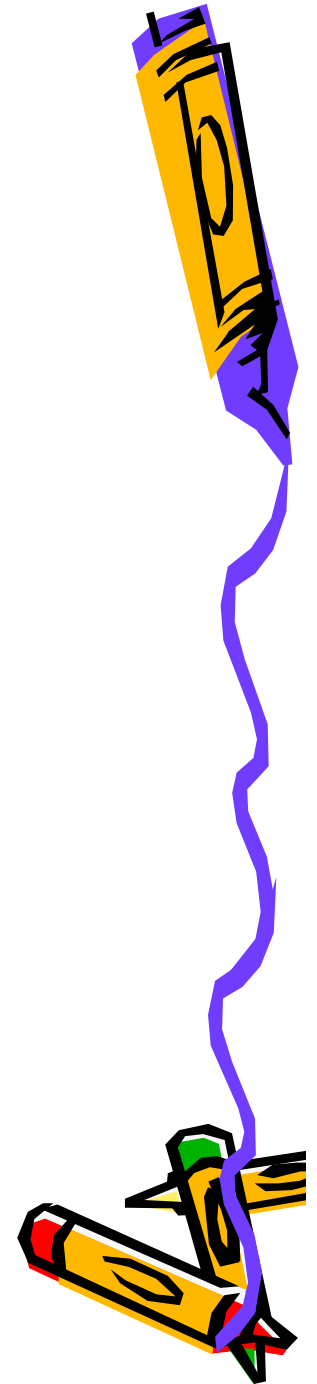
Req.0106 : Setup statistical test suites for most sensitive physics quantities

Responsible: J. Apostolakis, A. Ribon

Status:

- A first test suite for calorimetry quantities has been created. It measures longitudinal and lateral shower profiles for hadronics.
  - For several materials taken from LHC calorimeters.
- SLAC is continuously monitoring some variables most sensitive to BaBar and GLAST experiments.

Req.0303: Performance of G4

Responsible: J. Apostolakis / G. Cosmo

Description: "Compared to G3 simulation, under similar circumstances G4 is reported by the LHC experiments, to be a factor 1.5-2 slower. A study group started last year to address this issue, and should continue with more priority. This is expected to be a collaboration between G4 and the users."

Status

- Simple setup benchmarking is part of release process
- Propose regular meetings to address this issue, and other continuing issues (eg identifying hard to find problems).
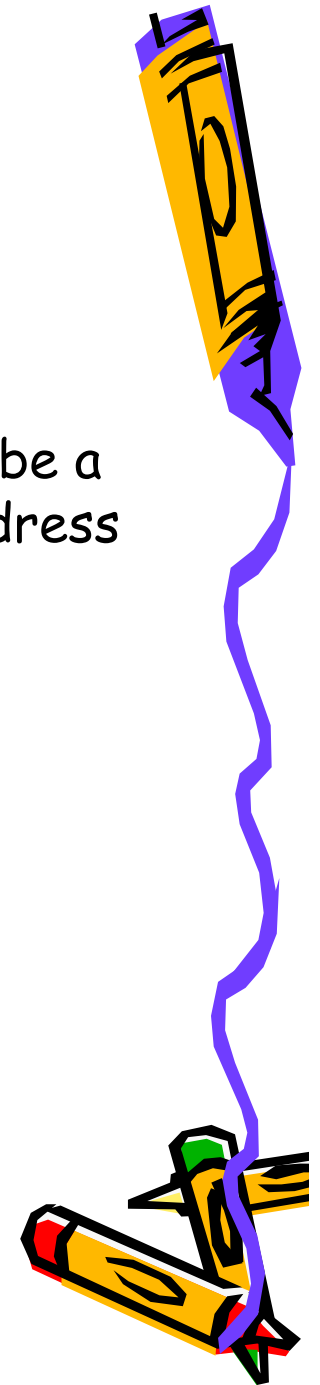
technical aspects of all available physics processes

Responsible: M. Maire / M.G. Pia / H.-P. Wellisch

Description: "All available physics processes, models, cross-sections, etc., should provide documentation of the technical aspects of the implementation: details of the expected behavior of a model should be provided (for example how incoming and outgoing particles are handled). This applies to both hadronic and electromagnetic processes."

- Concrete requirement for behavior of secondaries of hadronic process was fulfilled (Req.??).

- Physics group coordinators are open to suggestion of concrete issues and potential improvements.

Req.0401: Extension of Ion hadronics interaction to cover a good part of the cosmic ray range in (A,Z) and energy

Responsible: H.-P. Wellisch
Requestor: ESA (G. Santin)

- EM dissociation: Released in G4 6.2
- Inelastic reactions
  - Below 10 GeV per nucleon: Released Xsec in 6.0, extended models in 6.1 for light ions (<= C)
  - Above 10GeV/nucleon
    - Evaluated existing Xsec parameterisations – they are now good to about 20%. Extended QGSM to predict these Xsec and made a systematics of these predictions at O(1%) level.
    - Prototype extension of QGSM for final state generation in central rapidity for all ions and projectile and target fragmentation based on exciton pre-equilibrium model.
  - Work to be done: radioactive decay for relativistic ions, EM dissociation for higher excitations than quadropole resonance.
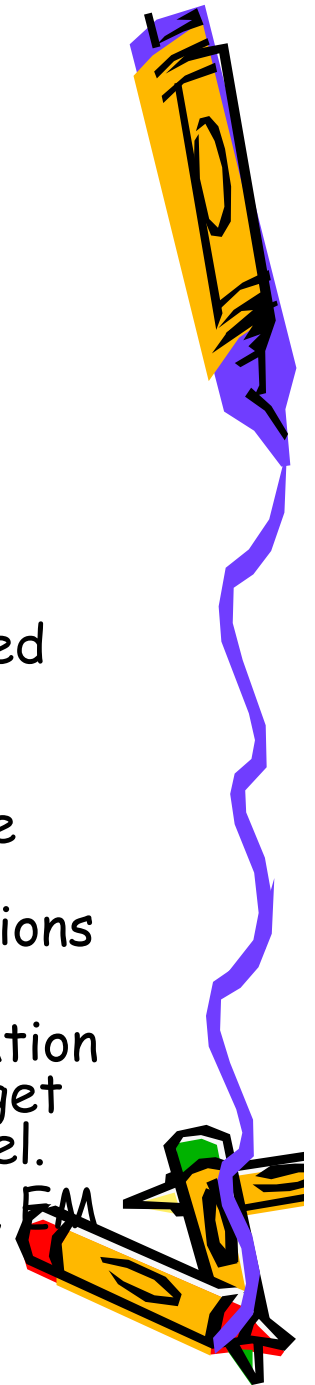
Req.0402: "Intuitive" documentation of the physics lists

Responsible: M. Maire / M.G. Pia / H.-P. Wellisch

Requestor: ESA (G. Santin)

Description: "Intuitive documentation (maybe in graphical form) for each physics list to show, for a given particle, which model is active over which energy range. It could also be printed out by the list in ASCII format, with a loop over inserted models."

Status

Hadronics: accepted, first prototype of 'model' directory circulated.

Req.0506: Optical photon transport in setups with repeated volumes

Responsible: P. Gumplinger

Requestor: TRIUMF (P. Gumplinger)

Enable optical photon transport in setups with parameterized/replicated/divided volume

Status

Revisions being prepared to enable use of 'replicated' volumes in optical processes.
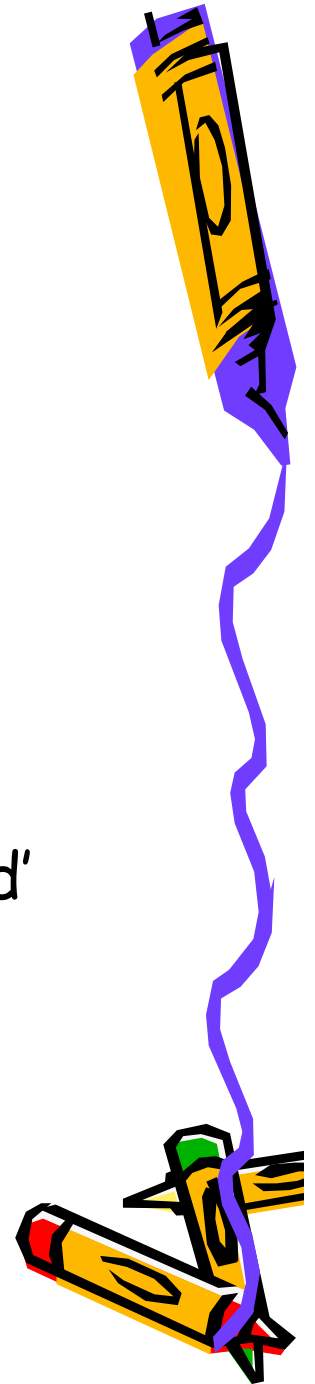
# 702. Selective verbosity

Originator: LHCb (G. Corti)

Responsible : T. Sasaki

- "We would like more configurable debugging features.
    - It is possible to follow in details various aspects of the simulation by setting verbose levels.
    - This is very hard to use when tracking complete pp events because millions of G4Track are produced.
- It would be very useful to be able to selectively turn on such verbose for a single G4Track, a single region of the detector, a combination of the two."
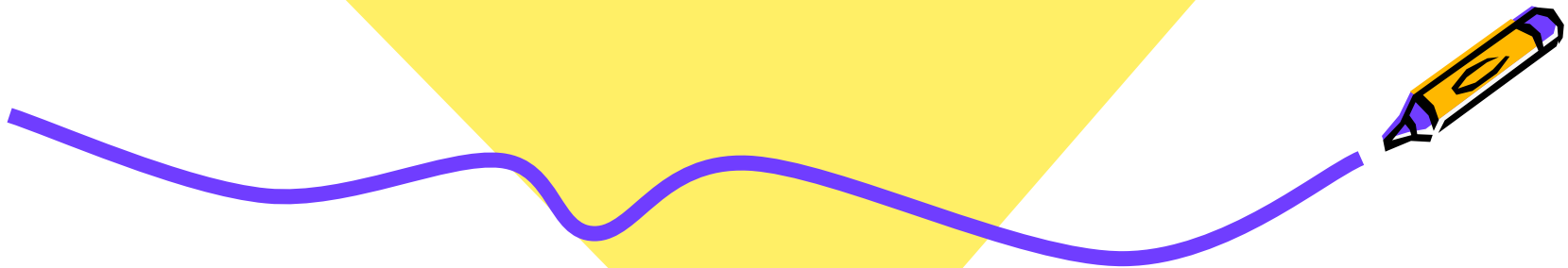
Status

- Feature is certainly desirable for debugging
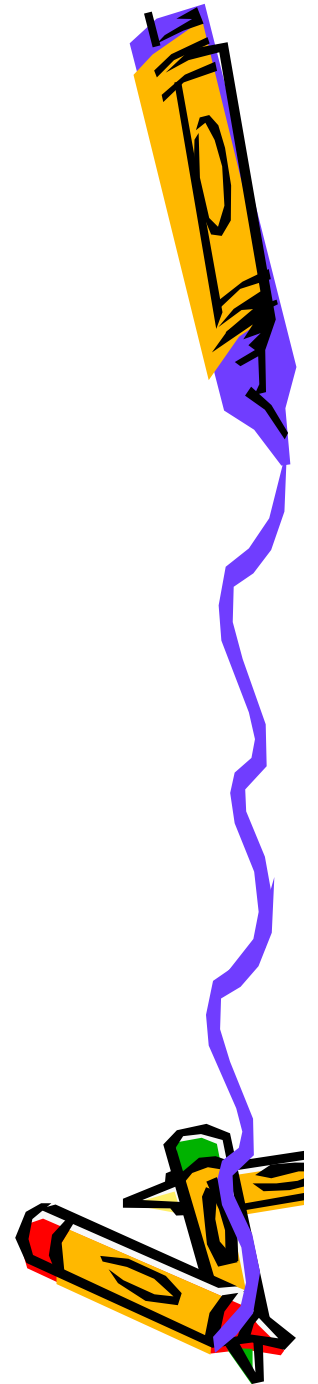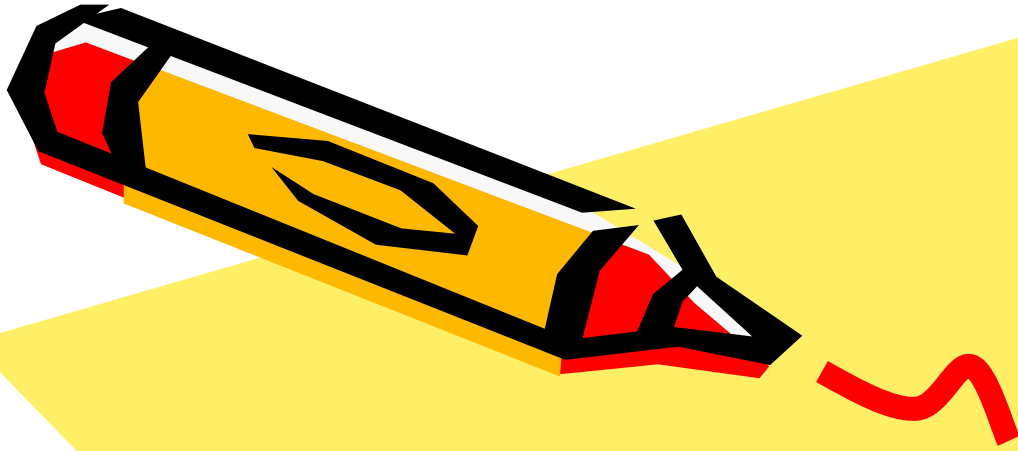- Currently seen as a long-term need, not urgent.
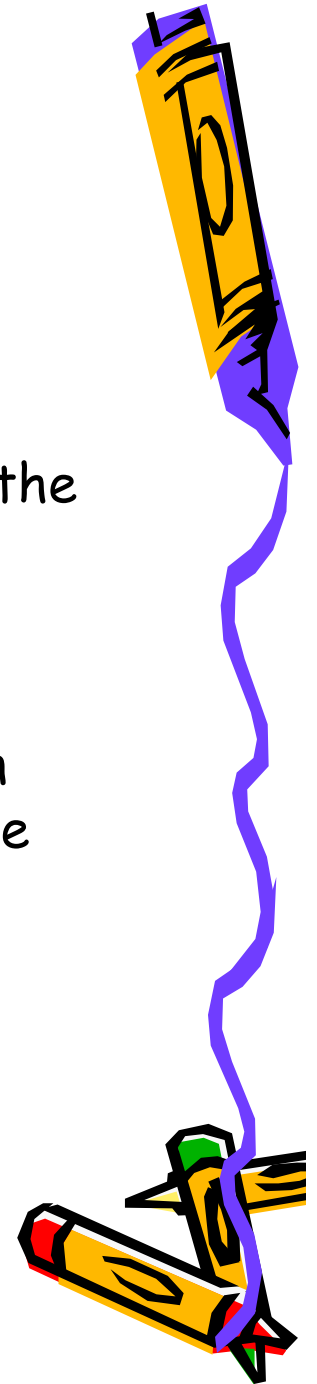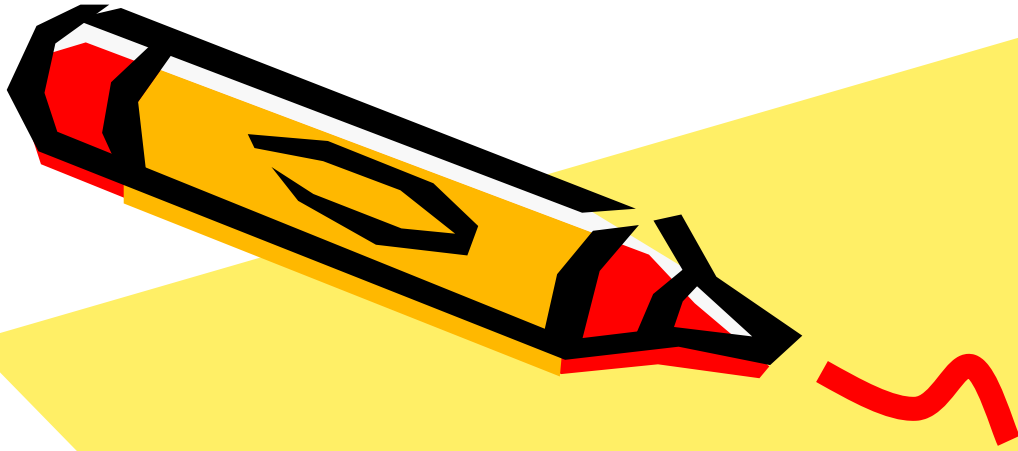
Requirements closed by
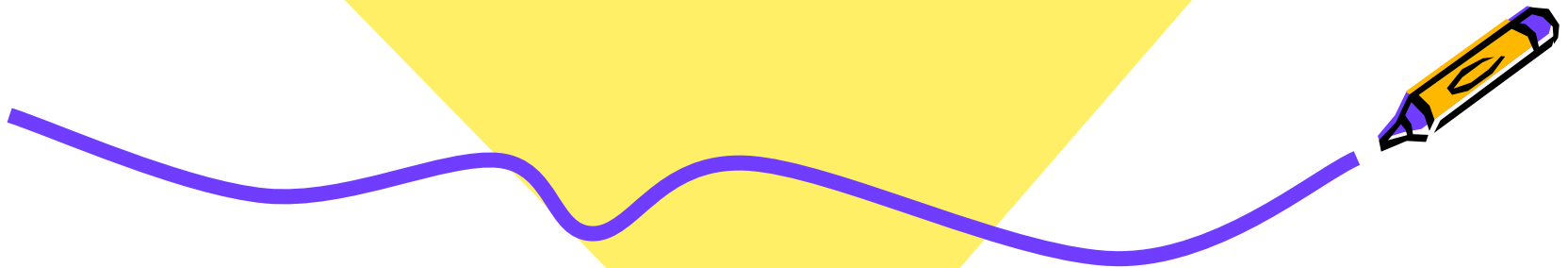December 2005

Requirements closed by G4 v7.1

- Req. 0701: Polarised Rayleigh scattering
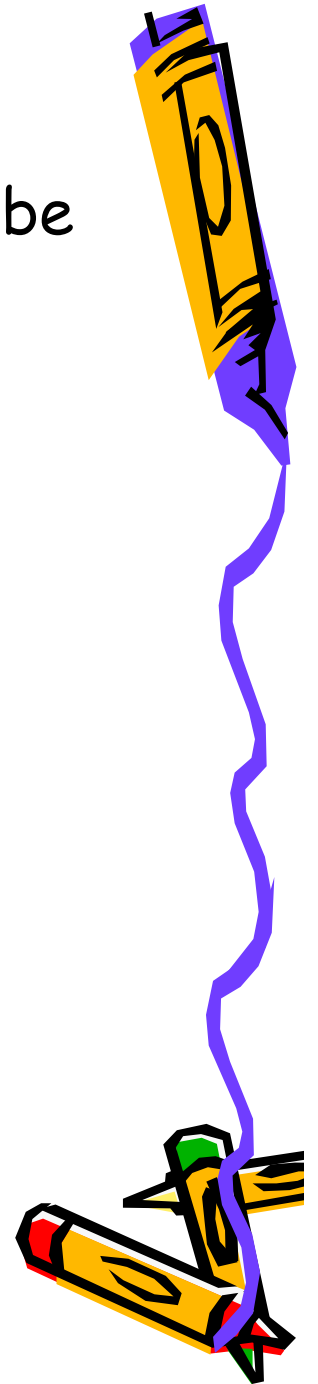- Req.0705: User Limits per region

- To be closed:

Requirements closed by
September 2005

Requirements closed by March 2005

- Req.0311: Parameters used in physics list should be well document and under user control.
- Req.0504: Geant4 release should be tested by Valgrind

Requirements closed by G4 v7.0

- Req.0208 : Enhanced saving and restoring of selected processes' cross-section tables AND Req.0306: Storage retrieval of cuts/physics-tables
- Req.0304: Exchange format for the geometry
- Req.0307: Region settings in reflected geometries
- Req.0312: Possibility of customizing volume/solid creation step
- Req.0503: Possibility of adding new particles for searches of new physics
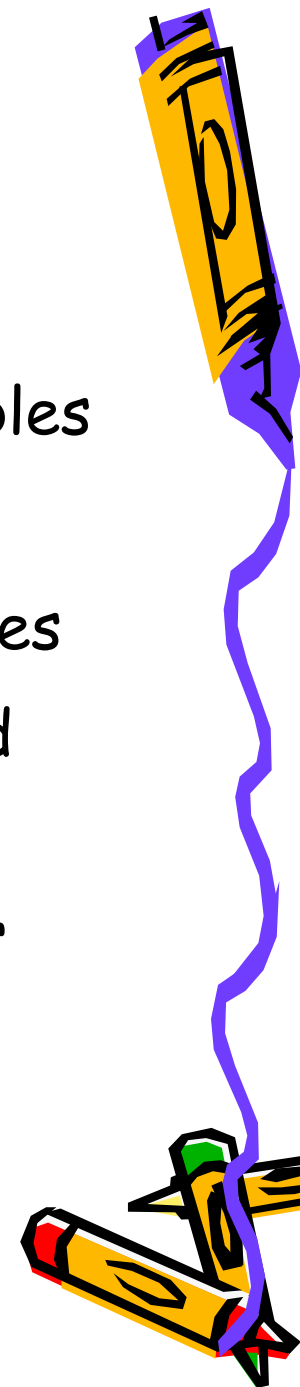
list should be well document and under user control

Responsible: H.-P. Wellisch

Description: "When the behavior of a specific physics list depends on parameters (for example on a momentum threshold) this should be clearly documented, specifying if such parameters are fixed or under user control."

- Note (from discussion): Major user modifications, such as these, would reduce the value of comparisons of the same physics list between users and experiments.
  - Physics list is free of user-tunable parameters except production thresholds.
- To be closed.
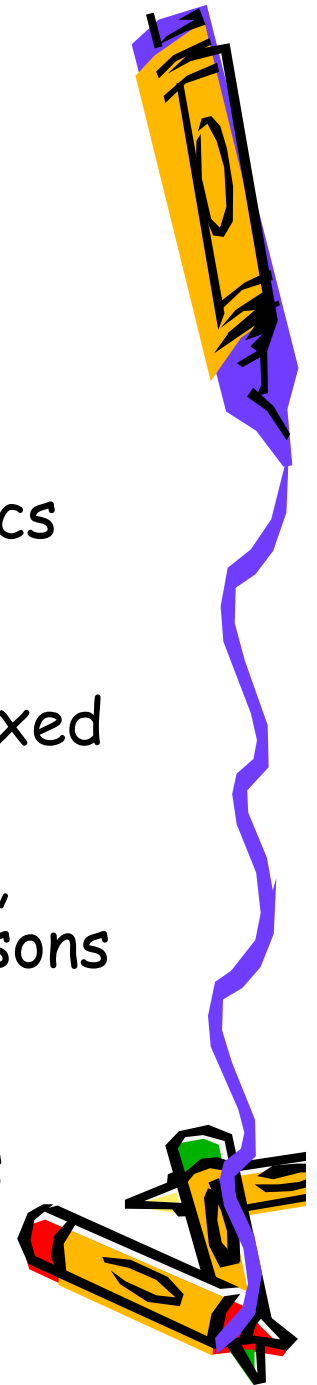
Req.0504: Geant4 release should be tested by Valgrind

Responsible: G. Cosmo, S. Sadilov

Requestor: LHCb

- Usage of Valgrind has been part of the release procedure since over two years
  - previously Insure++ was used for memory leaks & runtime error reports.
    - Selected system tests are checked.

Problems are reported to developers.

- Developers are requested to fix the reported problems
  - in particular those reported by Valgrind involving errors at runtime.
- To be closed.

Closed