Validation Strategies and Tools

Gunter Folger

Overview

- Validation and verification is performed by many
- I want to concentrate on validation:
  - How – what is the strategy of validating simulation of physics results
  - Tools – what tools are used
- Many other activities exist, these are not important, but will be ignored
  - Integration testing
  - Performance testing
  - Reproducibility
  - …

Validation strategy

There is no judgement intended in any of the slides

In collecting information from collaborators, I may have badly understood some answers, or ignored or skipped over some important aspects in the replies.

Albeit trying to be fair, I better know what is done in hadronics or EM compared to other fields

Method

- As a layman, ask the experts
- A small set of questions given to collaborators(*) involved in ongoing validation activities
    - Ignoring activities by developer of a process or model during development
    - Ignoring validations done by external groups
    - (*) Certainly incomplete list; only ~50% replies
  - Type of data used in validation, any selection, weights
  - How are validation jobs run
  - Tools to collect results or compare simulation to data
  - Frequency
  - ‘Publishing’ of results
  - Validation code in repository

Type of data used for validation

- Published experimental data: hadronics, standard EM, Medical (often contacting orginal authors)
- International recommendation: low energy EM
- In-house experimental data: Medical, low energy EM
- Published simulation results by other MC codes: low energy EM

- Datasets have equal weight – no explicit preference for specific experiments
  - Hadronics tries to identify more data with materials relevant in calorimetry over data using mostly light elements

Validation code

- Setup used
  - Thin target like, ~all
    - Both model and process level exist
  - Full setups ~all
- In repository ~ all
  - Test, examples both in use

Running validation

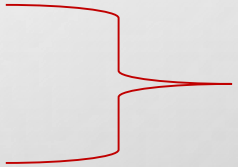
- Resources
  - Local machines/cluster: medical, low energy EM
  - Supercomputer: medical
  - batch/grid: EM, hadronics
- Frequency
  - Every reference tag: low energy EM, EM, hadronics – simplified calo, others if needed
  - Public release: all
- Automation:
  - Scripts used by all, and use of ranges from (semi)-automatic to fully automatic

Results

- Format:
  - (Root) plots: ~all
  - Numbers: low energy EM
- Comparison via
  - Statistical analysis, ratio plots: medical, EM, hadronics (thin target comparison)
  - Comparing plots/ numbers: low energy EM, hadronics (simplified calo)
- Report to collaboration: ~all,
  - Some reports also in regular working groups meetings, or other regular meetings
- Publish comparison (journal): medical, …

Use of tools

- Collection of results
  - Root macros
  - Automated publishing of results: EM, hadronics (in part)
- Storing/sharing of results
  - DoSSiER: hadronic thin target, cross section tests
  - Geant-val: hadronic simplified calo, some EM (activity starting)
  - Files with sharing of results: EM: AFS/EOS with web application to access plots
  - Files – no sharing of result: low energy EM, medical



Database with web interface

Regression of validation results

- Validation is run regularly in all physics areas
  - every reference tag or public release
- Tools to store and retrieve results used typically in HEP related activities
  - DoSSiER: used in validation of hadronic models, processes, and cross sections
    - Provides experimental data
  - Geant-val: used in validation of hadonic showers in calorimetry
    - Starts to be used for EM validation as well
  - EM validation tool - web interface to plots in file-system

Database with web interface

DoSSiER

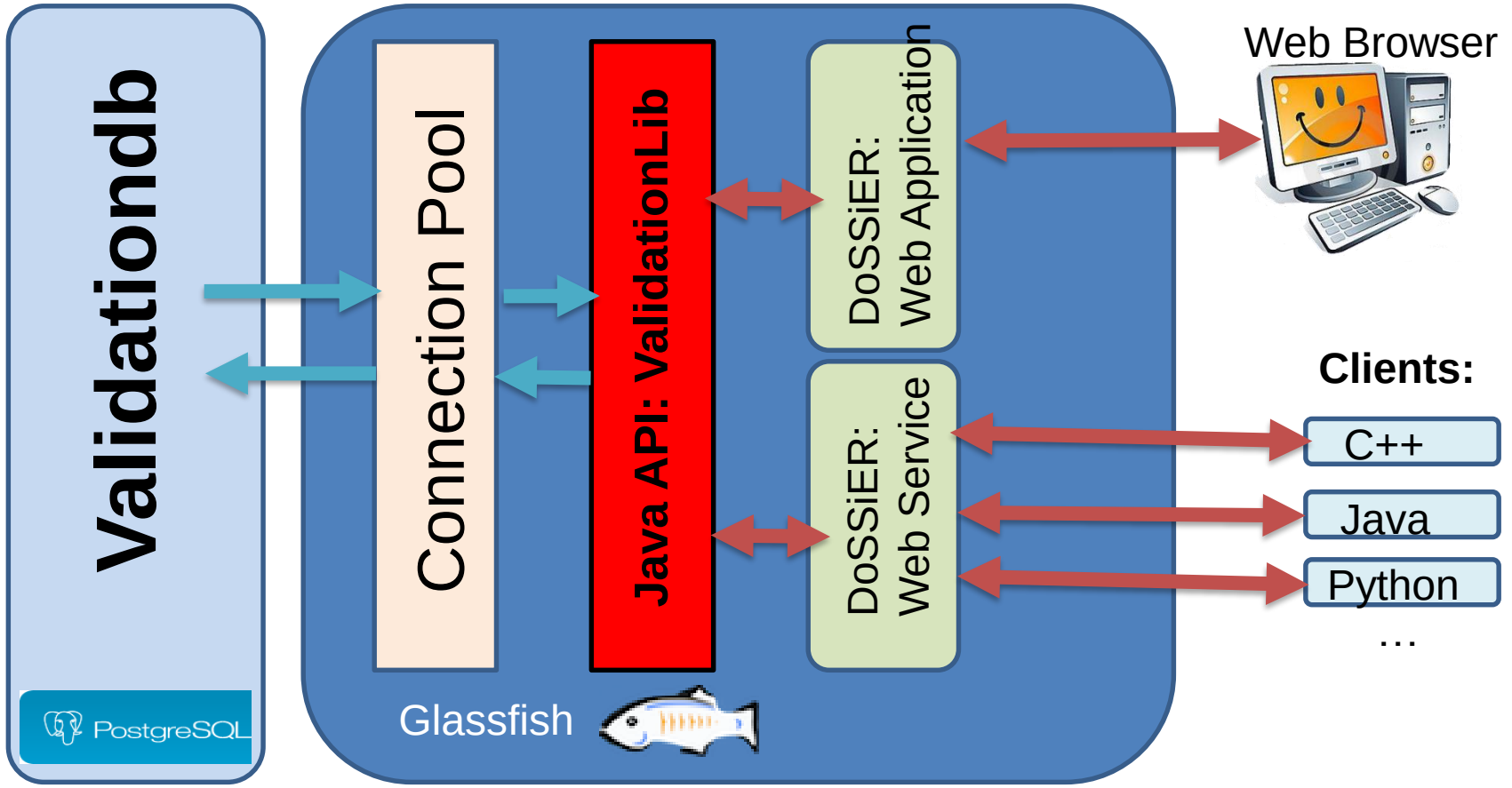
http://g4validation.fnal.gov:8080/DoSSiER/Welcome.xhtml

Slides contributed by Hans Wenzel

About DoSSiER

- Provides repository:
  - to store all experimental data used for Geant4 as raw data. (Currently ~ 4000 experimental data curves in db.). Data can be retrieved via web service.
  - to store simulation results as raw data and as static plots. (Currently ~200K simulated results in db.)
- Provides secure display web-application which:
  - allows to select and overlay compatible tests,
  - allows to overlay experimental data,
  - allows secure automatic upload into repository,
  - allows to display static images,
  - provides search functions and easy navigation.
- Provide REST-ful Web service which:
  - allows programmatic access to the data

Components



+ python ancillary tools: e.g. converter between various data formats: root, ascii, json to DoSSiER json format for upload. Uses Web Service to populate dictionaries.

Manpower

- Just a fraction of Hans time → mainly maintenance , migrating to new database servers and postgres version, bug fixes, very few mayor features implemented (human readable json files using keywords instead of link, consequent use of dictionaries..), adding new data (experimental and simulation)
- Julia, providing lots of data and feed back.
- Lost Andrea Dotti: he provided lot of feed back and was a great supporter, he provided python tools → Hans took over that task.
- CERN: decided to concentrate on their own tool.
- No summer student this year
- To do list is growing.

Geant4 Test Browser

As of Tue Aug 28 15:20:34 CDT 2018

Number of distinct Geant4 tests with results in database: 10

Number of data sets in database: 194428

Geant4 tests with Results in DoSSiER. Click on the ID to select Test

ID	Name	Description
10000	Franz	Neutron-induced production of protons, deuterons and tritons by neutrons between 300-580 MeV
48	test48	Stopping particle test Monte Carlo predictions are compared to experimental data.
2001	simplifiedCalo	Test of Shower shapes using selected simplified calorimeter setups.
10002	Pion Cross sections	Compare total,elastic,inelastic pion cross section with data
19	test19	High energy Experiment, provides comparison with NA61 (31 GeV/c proton beam) and NA49 (158 GeV/c proton beam) data sets.
10003	ProcessLevel	Process level (single interaction) validation test suite
23	test23	Physicslist label test.
41	test41	Validation of multiple and single Coulomb scattering of muons versus MuScat experimental data
75	test75	Test of gamma-nuclear interactions.
47	test47	Intermediate energy validation.

Sources of experimental data

- Existing databases:
  - HEPData: https://hepdata.net/
  - ExFor: http://www.nndc.bnl.gov/exfor/exfor.htm
  - Inspire: https://inspirehep.net/ -> cross link for references
  - Particle Data Group: http://pdg.lbl.gov/ (cross section, energy loss)
- Directly from article/thesis: if only paper copy OCR, engauge digitizer….
- Both e.g. geant4 or Genie developers have data collections.
- Experimental web sites: https://spshadrons.web.cern.ch/spshadrons/
- Compilations: https://www.oecd-nea.org/dbdata/bara.html
- Labor intensive and error prone, biased. Currently ~ 4000 experimental data curves in db.

Experiment Browser

As of Tue Aug 28 15:30:35 CDT 2018
Number of distinct experiments with results in database: 40
Number of data sets in database: 3913
Experiments with Results in the Database. Click on the ID to select the Experiment you are interested in, Click on link to find out more about the Experiment

ID	Title	Journal	Authors	Results	Link
44	Forward production of charged pions with incident pi+- on nuclear targets measured at the CERN PS	Nucl.Phys.**A821** (2009) , p: 118-192	Apollonio, M. et al.	384	link
45	Large-angle production of charged pions with incident pion beams on nuclear targets	Phys.Rev.**C80** (2009) , p: 065207	Apollonio, M. et al.	864	link
46	Forward production of charged pions with incident protons on nuclear targets at the CERN PS	Phys.Rev.**C80** (2009) , p: 035208	Apollonio, M. et al.	200	link
49	Measurements of Cross Sections and Charged Pion Spectra in Proton-Carbon Interactions at 31 GeV/c	Phys.Rev.**C84** (2011) , p: 034604	Abgrall, N et al.	20	link
50	Measurement of Production Properties of Positively Charged Kaons in Proton-Carbon Interactions at 31 GeV/c	Phys.Rev.**C85** (2012) , p: 035210	Abgrall, N. et al.	4	link
53	Detailed analysis of soft hadronic interactions	**(0) , p:**	NA49 et al.	232	link
56	Experimental Study of the a-Dependence of Inclusive Hadron Fragmentation	Phys.Rev.**D27** (1983) , p: 2580	Barton, D.S. et al.	90	link
57	Measurements of the proton total reaction cross section for light nuclei between 20 and 48 MeV	Phys.Rev.**C10** (1974) , p: 2237-2246	Cameron, J.M. et al.	5	link
68	Measurement of Neutron-Production Double-Differential Cross Sections for Nuclear Spallation Reaction Induced by 0.8, 1.5 and 3.0 GeV Protons	J.Nucl.Sci.Technol.**34** (1997) , p: 529-537	CHIBA, Satoshi et al.	76	link
69	Measurements of $\pi ^{\pm }$, $K^{\pm }$, K^0_S , $\varLambda $ and proton production in proton–carbon interactions at 31 GeV/c with the NA61/SHINE spectrometer at the CERN SPS	Eur.Phys.J.**C76** (2016) , p: 84	Abgrall, N. et al.	63	link
70	Barashenkov Compilation of cross sections for nucleon induced reactions at energies above a few MeV.	**(0) , p:**	Barashenkov B.C. et al.	296	link
71	The scattering of muons in low Z materials	Nucl.Instrum.Meth.**B251** (2006) , p: 41-55	Attwood, D. et al.	10	link
72	Weak radiative decay Lambda ---> n gamma and the radiative capture reaction K- p ---> Sigma (1385) gamma.	Phys.Rev.**D47** (1993) , p: 799-810	Bassalleck, B. et al.	1	link
74	Low-energy anti-proton physics	Ann.Rev.Nucl.Part.Sci.**41** (1991) , p: 219-267	Amsler, Claude et al.	1	link
75					

Etc.....

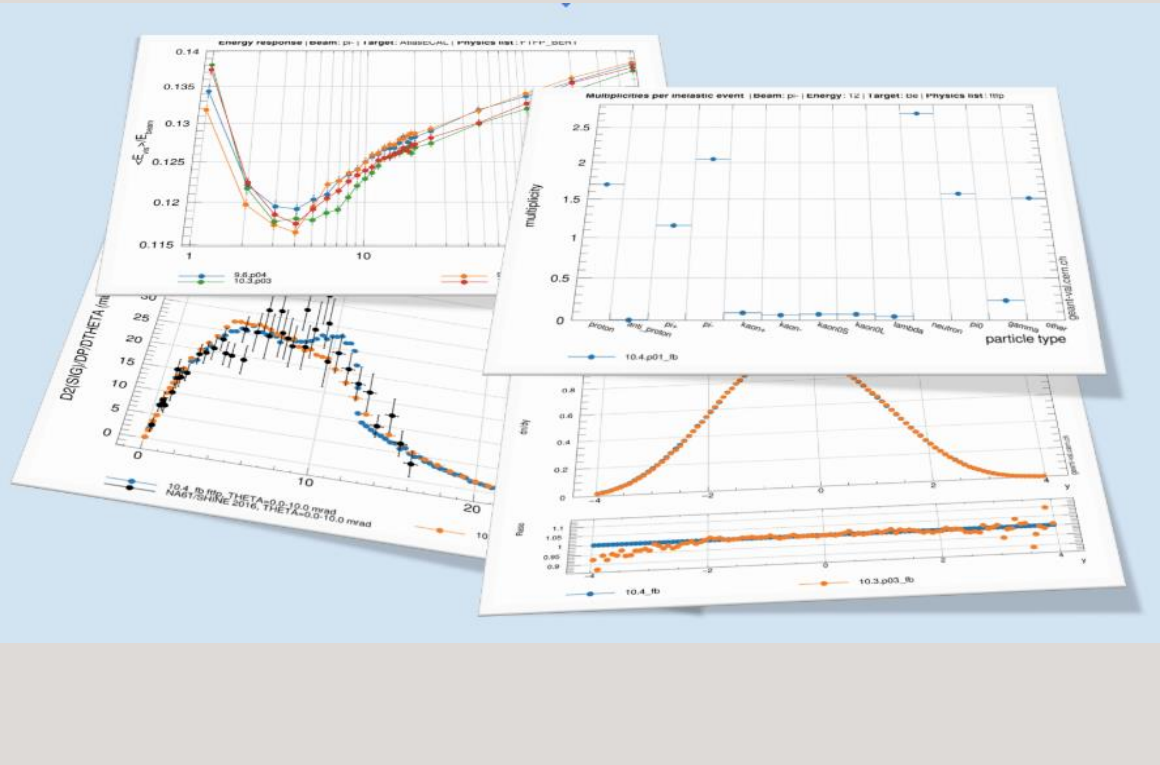
Geant-val

https://geant-val.cern.ch/

Slides contributed by Dmitri Konstantinov

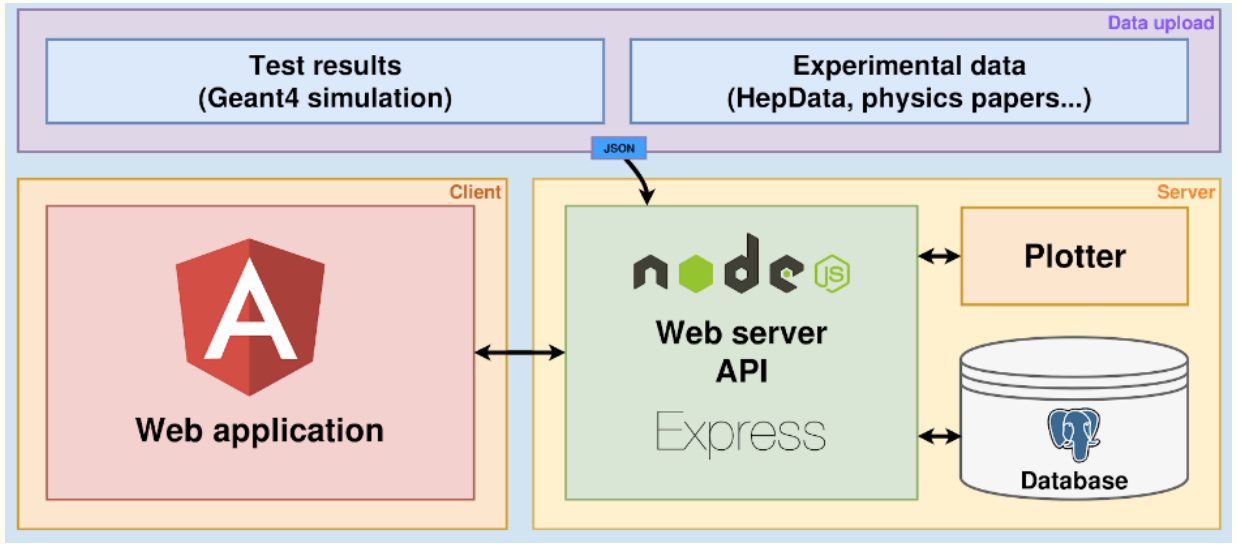
GEANT-VAL:
VALIDATION WEB APPLICATION
(+ USEFUL SIDE PRODUCTS)

Luc Freyermuth — ESTI, France
Dmitri Konstantinov — IHEP, Protvino
Grigory Latyshev — IHEP, Protvino
Ivan Razumov — IHEP/CERN



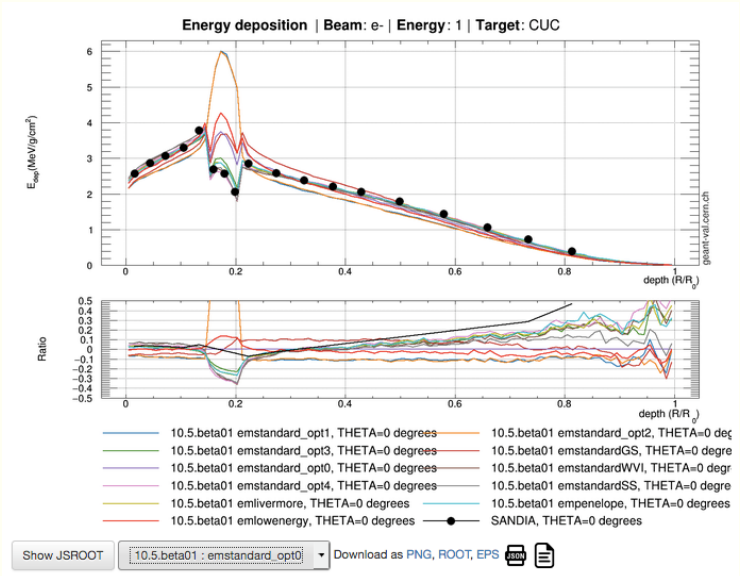
Introduction

- The CERN/SFT group, which contributes to the development, testing, deployment and support of the toolkit, is also in charge of monthly running a set community-developed tests using the development releases of Geant4.
- We developed the Web application "geant-val" for visualizing results of these tests and comparing them between different Geant4 releases. The application is written using Express.js, Node.js and AngularJS framework, and uses PostgreSQL for storing test results.



What “geant-val” can

- allows visual plots comparison using overlaying and ratio plots
  - Release with release
  - Release with experimental data
  - Physics models/physics lists
- allows to perform statistical comparison of test results
- displays static PNG plots (better quality) and interactive plots using JSROOT
- allows to download plots in PNG, ROOT and EPS formats
- allows to download input histograms in JSON and GNUplot formats



User layouts - https://geant-val.cern.ch/layout

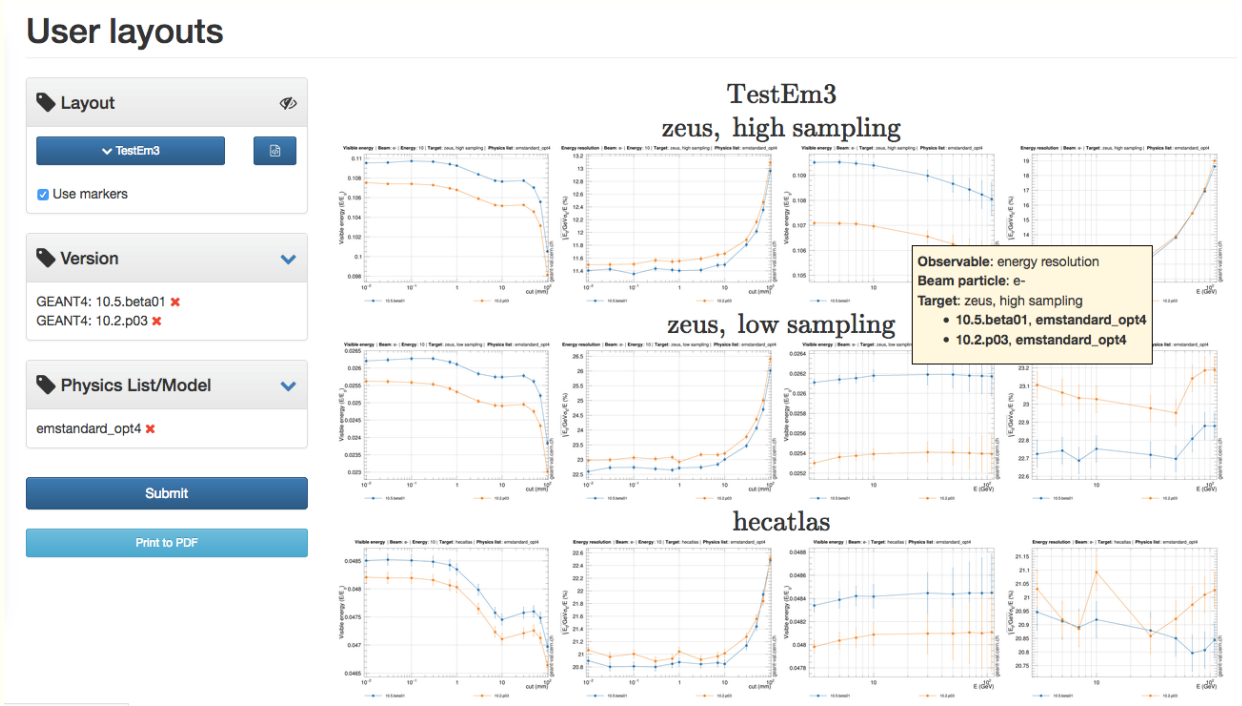
TestEm3.xml 3.47 KB Edit | Web IDE | Replace | Delete

```
<?xml version="1.0" encoding="UTF-8"?>
<layout>
  <default model="emstandard_opt0"></default>
  <row>
  <label text="\LARGE{TestEm3}" colspan="4"/>
  </row>

  <row><label text="\LARGE{zeus, high sampling}" colspan="4"/></row>
  <row>
    <plot test="TestEm3-cutTest" observable="visible energy"    beam="e-" energy="10" secondary="None" target="zeus, high sampling" yaxis="lin" xaxis="log"
    <plot test="TestEm3-cutTest" observable="energy resolution" beam="e-" energy="10" secondary="None" target="zeus, high sampling" yaxis="lin" xaxis="log"
    <plot test="TestEm3-Energy" observable="visible energy"    beam="e-" energy="MULTIPLE" secondary="None" target="zeus, high sampling" yaxis="lin" xaxis="
    <plot test="TestEm3-Energy" observable="energy resolution" beam="e-" energy="MULTIPLE" secondary="None" target="zeus, high sampling" yaxis="lin" xaxis="
  </row>

  <row><label text="\LARGE{zeus, low sampling}" colspan="4"/></row>
  <row>
    <plot test="TestEm3-cutTest" observable="visible energy"    beam="e-" energy="10" secondary="None" target="zeus, low sampling" yaxis="lin" xaxis="log" t
    <plot test="TestEm3-cutTest" observable="energy resolution" beam="e-" energy="10" secondary="None" target="zeus, low sampling" yaxis="lin" xaxis="log" t
    <plot test="TestEm3-Energy" observable="visible energy"    beam="e-" energy="MULTIPLE" secondary="None" target="zeus, low sampling" yaxis="lin" xaxis="l
    <plot test="TestEm3-Energy" observable="energy resolution" beam="e-" energy="MULTIPLE" secondary="None" target="zeus, low sampling" yaxis="lin" xaxis="l
  </row>

  <row><label text="\LARGE{hecatlas}" colspan="4"/></row>
  <row>
    <plot test="TestEm3-cutTest" observable="visible energy"    beam="e-" energy="10" secondary="None" target="hecatlas" yaxis="lin" xaxis="log" title=""/>
    <plot test="TestEm3-cutTest" observable="energy resolution" beam="e-" energy="10" secondary="None" target="hecatlas" yaxis="lin" xaxis="log" title=""/>
    <plot test="TestEm3-Energy" observable="visible energy"    beam="e-" energy="MULTIPLE" secondary="None" target="hecatlas" yaxis="lin" xaxis="log" title=
    <plot test="TestEm3-Energy" observable="energy resolution" beam="e-" energy="MULTIPLE" secondary="None" target="hecatlas" yaxis="lin" xaxis="log" title=
  </row>
```



User-defined layouts can be used for fast visual validation of Geant4. User can define their own XML template to show the plots in the layout they want.. Some predefined templates are already available in the application.

Statistical comparison

χ^2 and Kolmogorov-Smirnov statistical tests allows test results for **different** versions of Geant4 to be compared. The calculations are performed on the client side using JavaScript workers.

Stat comparison

TestEm9

filter menu entries
visual mode
ROOT plots JSROOT plots

Version
10.4.ref07
10.5.beta01

Beam
e-

Observable
Default group (Deselect all)
energy resolution 1x1
energy resolution 3x3
energy resolution 5x5
visible energy 1x1
visible energy 3x3
visible energy 5x5

Deselect all observables

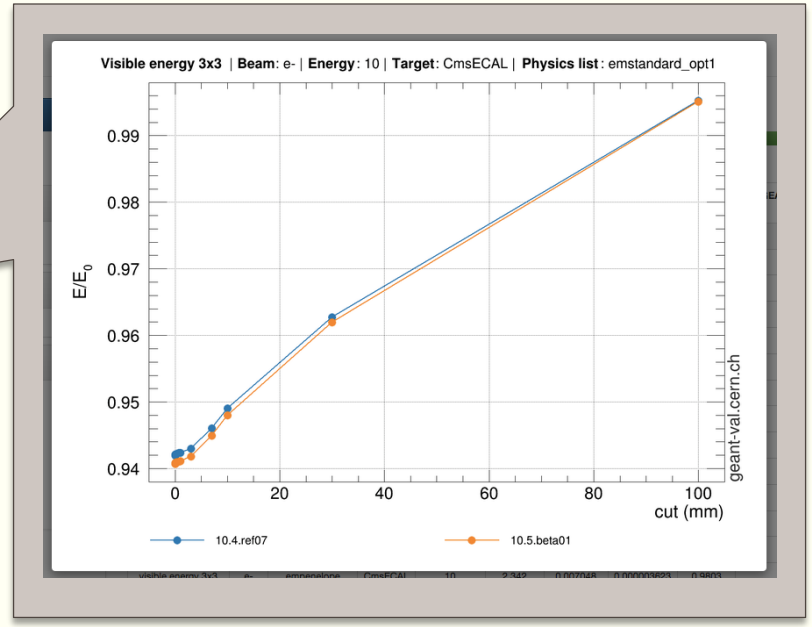
Submit

Statistical tests

48 / 48

$< \chi^2 >= 100.16 \pm 428.82; \sum_1^{48} \chi^2 = 4807.89$

Observable	Beam	Model	Target	Beam energy	χ^2/NDF	χ^2 Prob	KS max(D)	KS Prob	GEANT4: 10.4.ref07 with GEANT4: 10.5.beta01	Image
visible energy 3x3	e-	emstandard_opt1	CmsECAL	10	2283	0	0.0001228	0	272266 and 273993	
visible energy 5x5	e-	emstandard_opt1	CmsECAL	10	1958	0	0.00008064	0	272269 and 273997	
visible energy 1x1	e-	emstandard_opt1	CmsECAL	10	512	0	0.0001571	0	272271 and 273999	
visible energy 3x3	e-	emlowenergy	CmsECAL	10	6.52	5.756e-11	0.00001676	0.0002165	272272 and 273951	
visible energy 1x1	e-	emlowenergy	CmsECAL	10	4.847	1.575e-7	0.00002877	0.02446	272278 and 274000	
visible energy 1x1	e-	emstandard_opt4	CmsECAL	10	3.908	0.0000109	0.00001078	0.9227	272245 and 273953	
visible energy 3x3	e-	emstandard_opt4	CmsECAL	10	3.729	0.00002396	0.000005243	0.7803	272287 and 274001	
visible energy 1x1	e-	emstandard_opt2	CmsECAL	10	3.371	0.0001116	0.00001907	0.2681	272258 and 273979	
visible energy 3x3	e-	emstandard_opt2	CmsECAL	10	3.314	0.0001423	0.000006435	0.4844	272252 and 273974	
visible energy 5x5	e-	emlowenergy	CmsECAL	10	3.051	0.0004273	0.000004527	0.4591	272275 and 273984	
visible energy 3x3	e-	emstandard_opt3	CmsECAL	10	2.492	0.003978	0.000008608	0.1688	272243 and 273960	
visible energy 1x1	e-	emlivermore	CmsECAL	10	2.454	0.004606	0.00002866	0.02038	272251 and 273959	
visible energy 1x1	e-	emstandard_opt3	CmsECAL	10	2.411	0.005435	0.00002082	0.1793	272286 and 273966	
visible energy 3x3	e-	empenelope	CmsECAL	10	2.342	0.007048	0.000003623	0.9803	272259 and 273987	
visible energy 5x5	e-	emstandard_opt3	CmsECAL	10	2.297	0.00832	0.000005526	0.2277	272276 and 273964	
visible energy 1x1	e-	empenelope	CmsECAL	10	1.988	0.02544	0.00001306	0.7387	272264 and 273992	



Geant-config-generator

Geant-config-generator is Python-based utility managing user's physics tests:

- is a side product of **geant-val** development
- facilitates and makes more transparent the creation of test configurations from test configuration template and steering file.
- submits jobs to batch systems(CERN LSF and HTCondor).
- parses and combine produced results.
- creates input JSON files for **geant-val**.

```
#verbose
0
//            proton pi- pi+ kaon+ kaon- anti_proton
#particle
%PARTICLE%
//
#material
%MATERIAL%
#targetA
%TARGETA%
//            ftfp ftfb qgsp qgsb bertini binary
#generator
%GENERATOR%
//
#events
%NEVENTS%
//
//--------
#Plab(GeV/c)
%ENERGY%
#run
#exit
```

params.conf 582 Bytes

```
1  ! PARTICLE=proton, pi+, pi-
2  ! ENERGY=3.0,5.0,8.0,12.0
3  ! GENERATOR=ftfp
4  !CONST:ENERGY_UNIT=GeV
5  PARTICLE | ENERGY | MATERIAL | TARGETA | GENERATOR | NEVENTS
6  PARTICLE | ENERGY |  G4_Pb   | 208     | GENERATOR | 2000000
7  PARTICLE | ENERGY |  G4_Ta   | 181     | GENERATOR | 2000000
8  PARTICLE | ENERGY |  G4_Sn   | 119     | GENERATOR | 2000000
9  PARTICLE | ENERGY |  G4_Al   |  27     | GENERATOR | 2000000
10 PARTICLE | ENERGY |  G4_Cu   |  64     | GENERATOR | 2000000
11 PARTICLE | ENERGY |  G4_C    |  12     | GENERATOR | 2000000
12 PARTICLE | ENERGY |  G4_Be   |   9     | GENERATOR | 2000000
```

Tests integrated into **geant-val**

Test name	Project	Author	Description
FluctTest	GEANT4	Vladimir Ivanchenko	Example for investigation of G4 fluctuation models is on the base of TestEm8 (ionisation in thin absorbers and gaseous detectors). Simulation data are ... Show more
MscHanson	GEANT4	Vladimir Ivanchenko	The tests simulates multiple scattering distributions of 15.7 MeV electrons transmitted through thin foils of the indicated materials.
TestEm3-Energy	GEANT4	Vladimir Ivanchenko	TestEm3 simulates energy resolution and visible energy in hecatlas, zeus calorimeters
TestEm3-cutTest	GEANT4	Vladimir Ivanchenko	TestEm3 produces plots showing impact of production cut on energy resolution and visible energy
TestEm9	GEANT4	Vladimir Ivanchenko	TestEm9
hadr00	GEANT4	Vladimir Ivanchenko	Application demonstrating Geant4 hadronic cross sections
simplified calorimeter	GEANT4	Andrea Dotti, Alberto Ribon	The simulation program is implemented as a simplified geometry of sampling calorimeters. The calorimeter geometry consists of a cylinder with a radius ... Show more
test15	GEANT4	Alexander Howard	Comparison of Geant4 simulation against the TARC experiment. This test is a validation of the production, transportation and interaction of neutrons ... Show more
test22-HARP	GEANT4	Vladimir Uzhinsky	Double-differential proton production cross sections in the proton momentum range 0 to 8 GeV at angles 0.05 to 0.25 radians from collisions of charged ... Show more
test22-NA49	GEANT4	Vladimir Ivanchenko	
test22-NA61	GEANT4	Vladimir Uzhinsky	double differential PI+, PI-, proton production cross section in the laboratory system for p+C interactions at 31 GeV/c in different polar angle ... Show more
test37	GEANT4	Vladimir Ivanchenko	test37
test46	GEANT4	Vladimir Ivanchenko	Simulation of simplified combined calorimeter. Crystal electromagnetic (ECAL) calorimeter and sampling hadronic calorimeter (HCAL) are ... Show more
tileatlas	GEANT4	Vladimir Ivanchenko	tileatlas
main02	Pythia8		

"Integrated" – test can be run and results can be obtained using geant-config-generator

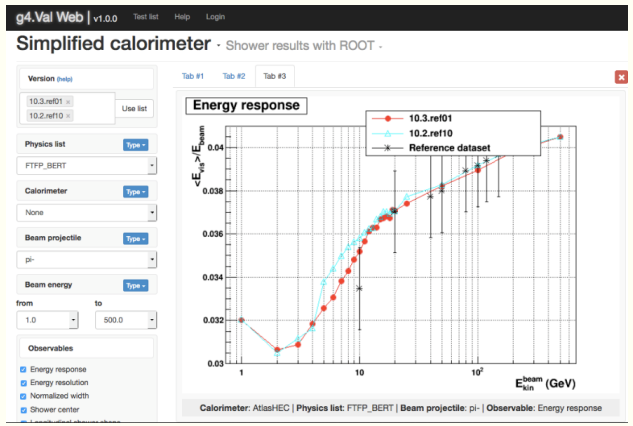
Summary

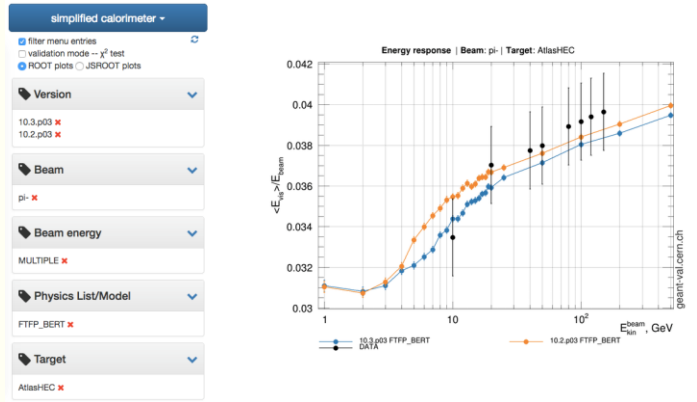
- Validation for HEP seems most advanced
  - Results available via web
- Low energy EM also does regular validation, results less accessible
- Validation for medical applications reported at workshops
  - How to establish better communication with physics working groups?
- Nuclear physics, space, … ?
- Have two validation DBs with web interface, focus differs

Backup

History

- **2013**: first validation page **g4-val** was created by G.Lestaris (CERN technical student), aimed to facilitate "hadronic physics" validation by CERN Geant4 group based on DJANGO, MySQL.
- **2016**: I.Ifrim (CERN summer student) has developed a prototype **geant-val** based on Node.js and AngularJS as "interface" to postgresql database of **DOSSIER** project.
- **2017**: After extensive development **geant-val** became production web application used by CERN "hadronic" group.
- **2017-2018**: A lot of improvements and many new features.





geant-config-generator

[Step 1] **Clone repo**

```
git clone ssh://git@gitlab.cern.ch:7999/GeantValidation/geant-config-generator.git
Cloning into 'geant-config-generator'...
```

[Step 2] **Submit jobs**

```
./mc-config-generator.py generate -t geant4/test37 -v 10.5.beta01 -q 1nd -r
Prepared 594 jobs for test test37.
Continue sumbitting in batch [y|n]?
Job <192600064> is submitted to queue <1nd>.
Job <192600065> is submitted to queue <1nd>.
Job <192600067> is submitted to queue <1nd>.
.........................
```

[Step 2.1] **Check status**

```
./mc-config-generator.py status -t geant4/test37 -d OUTPUT/
 == Geant4 10.5.beta01
  Test: test37
    Failed: 120
    Running: 296
    Pending: 178
    Total: 594
```

[Step 3] **convert/parse results to input geant-val JSON**

```
./mc-config-generator.py parse -t geant4/test37 -d OUTPUT/
```

[Step 4] **Upload JSONs to geant-val**

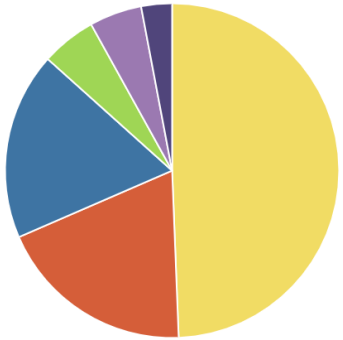
```
python geant_upload.py --krb -j OUTPUTJSON/geant4/10.5.beta01/x86_64-slc6-gcc49-opt/test37/*
```

geant-val repository statistics

geant-val

Programming languages used in this repository

JavaScript	49.37 %
HTML	19.12 %
Python	18.13 %
Shell	5.31 %
PLpgSQL	5.08 %
CSS	2.98 %



Commit statistics for master Aug 30 - Aug 26

master

GVP

- Total: **1699 commits**
- Average per day: **2 commits**
- Authors: **21**

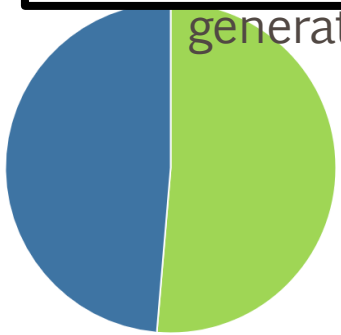
Commits per day of month

100

geant-config-generator

Programming languages used in this repository

Shell	51.34 %
Python	48.66 %



Commit statistics for master Oct 09 - Aug 22

master

geant-config-generator

- Total: **461 commits**
- Average per day: **1 commits**
- Authors: **4**

Commits per day of month

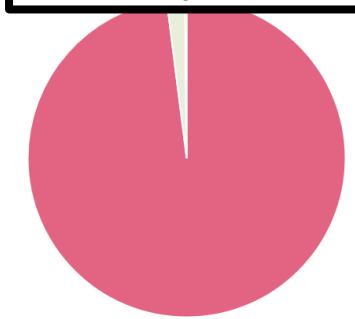
50

40

plotter

Programming languages used in this repository

C++	97.98 %
CMake	1.85 %
Shell	0.16 %



Commit statistics for master Mar 21 - Aug 26

master

plotter

- Total: **294 commits**
- Average per day: **0 commits**
- Authors: **8**

Commits per day of month

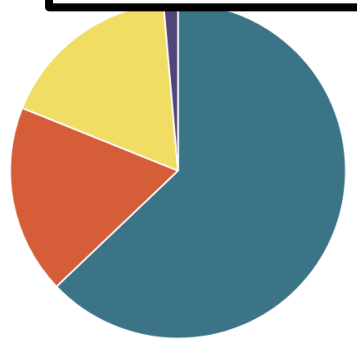
30

25

R&D (new)

Programming languages used in this repository

TypeScript	62.88 %
HTML	18.21 %
JavaScript	17.53 %
CSS	1.38 %



Commit statistics for master Jul 16 - Aug 27

master

Loopback

- Total: **397 commits**
- Average per day: **9 commits**
- Authors: **5**

Commits per day of month

50

40

Ongoing R&D

Motivation:

- In January 2018, a schedule was announced for phasing-out AngularJS: after releasing 1.7.0, the active development on AngularJS will continue till June 30, 2018. Afterwards, 1.7 will be supported till June 30, 2021 as long-term support.
- “hard-coded” parameters in database schema (“beam particle”, “beam energy”, “model”, “secondary particle”) limit web app usage to fixed target tests.

R&D:

- To try “parameter free” db schema
- To get experience with Angular

Conclusion

We have developed a web application **geant-val** facilitating validation of Geant4 which:

- have **intuitive user interface**
- have **nice graphics**
- Is **secure**

Which works and provides:

- **consistent storage of test results**
- **overlaying plots and ratio plots for regression testing**
- **possibility for comparison with experimental data**
- **simple statistical evaluation for regression testing**