

Update of Physics Vectors and global functions



V.Ivanchenko, CERN & G4AI

18th Geant4 Collaboration Workshop
23-27 September 2013
Sevilla, Spain

Introduction



Outline

- Fast mathematical functions
- Data vectors

Motivation from CPU profiling:

- significant contribution of standard library (log, exp, sincos .. – decenting order)
- Significant contribution of data access methods for cross section computations

MT migration required design change of data classes

G4Pow



- Initially this class was created in order to provide super fast values of frequently used functions of integer arguments Z and A
 - Z, A may vary from 1 to 512
- With time number of G4Pow methods increased
 - Additions were needed for PreCompound/DeExcitation models and cross sections
 - Fast computations with double arguments were also added, in particular, for fast computing of cross sections

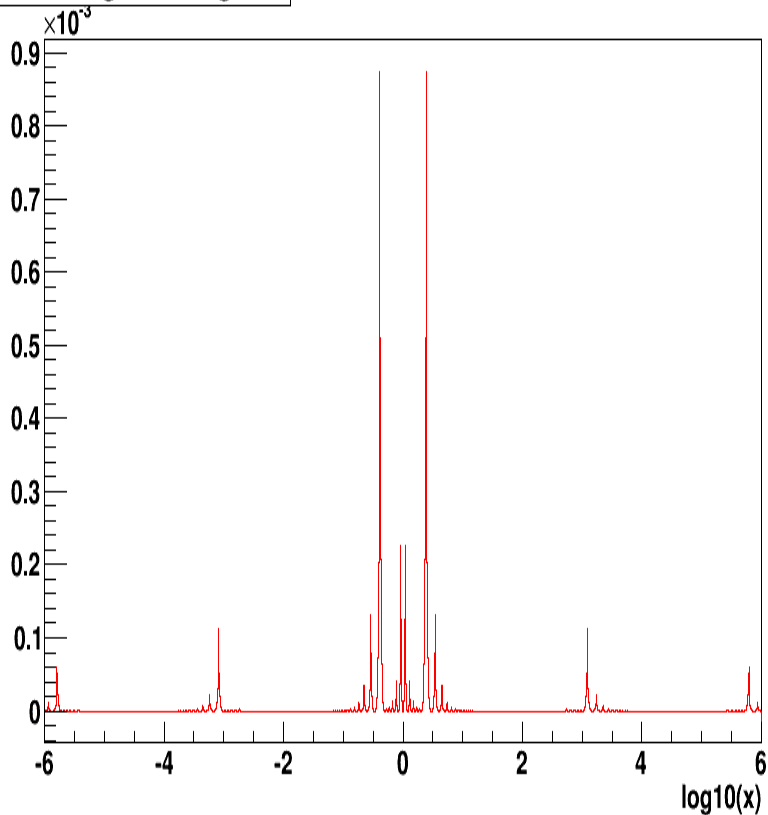
G4Pow



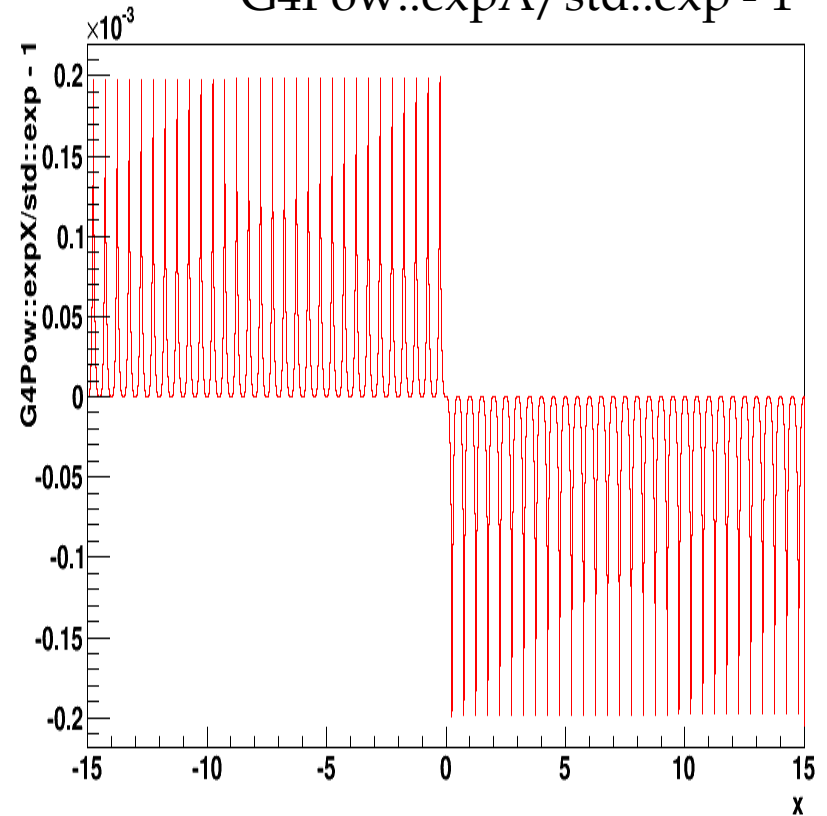
- ❧ Currently it is G4ThreadLocal singleton
 - ❧ I would propose to make it global singleton
- ❧ Current methods with integer arguments:
 - Z13(G4int)
 - Z23(G4int)
 - logZ(G4int)
 - log10Z(G4int)
 - powZ(G4int, G4double)
 - factorial(G4int)
 - Logfactorial(G4int)
- ❧ Current methods with double arguments:
 - A13(G4double)
 - A23(G4double)
 - logA(G4double)
 - logX(G4double)
 - log10A(G4double)
 - expA(G4double)

Accuracy of G4Pow::logX and G4Pow::expA

G4Pow::logX/std::log - 1



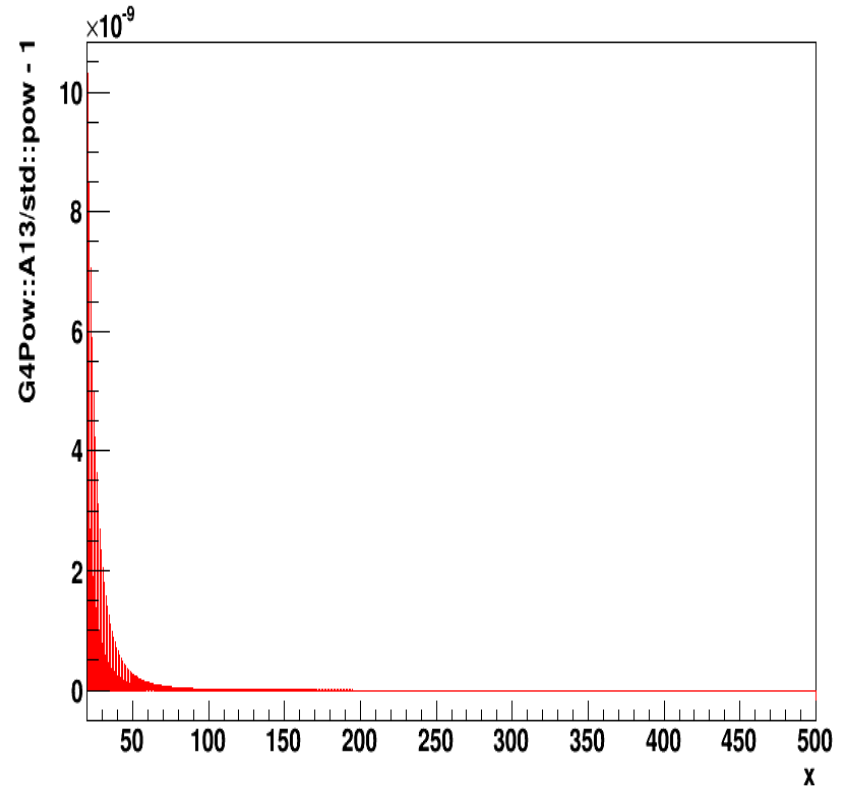
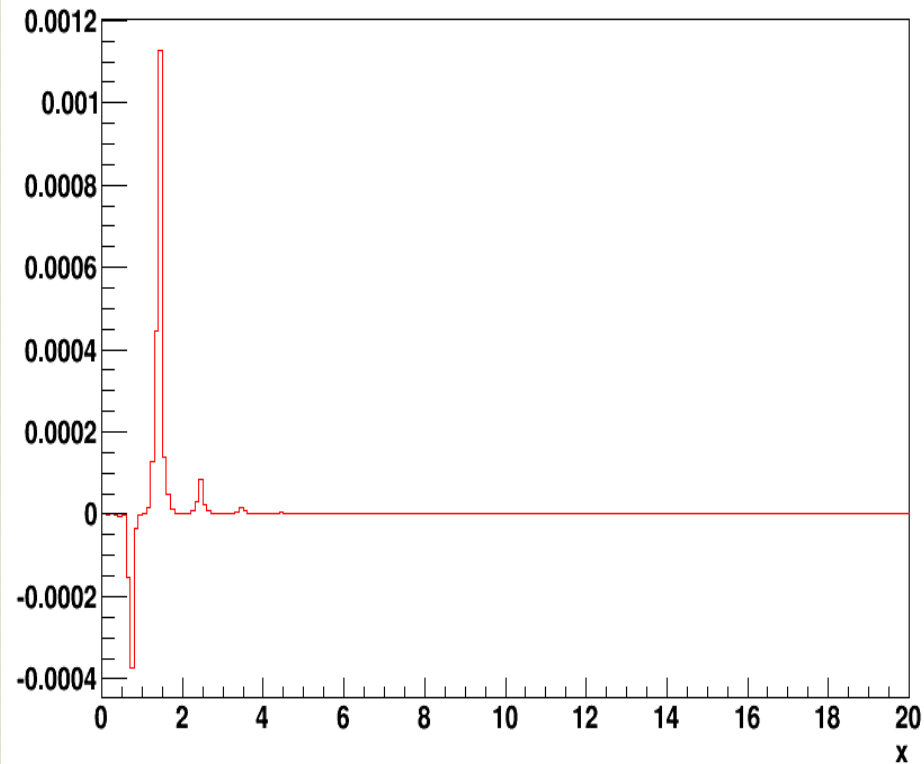
G4Pow::expA/std::exp - 1



Accuracy of G4Pow::A13



G4Pow::A13/std::pow - 1

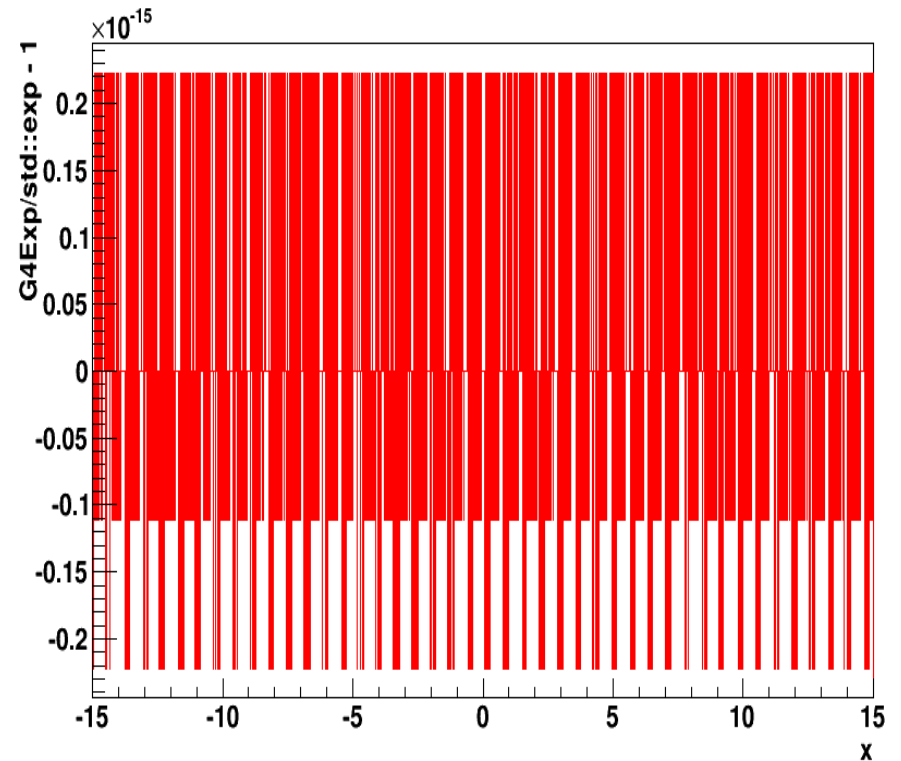
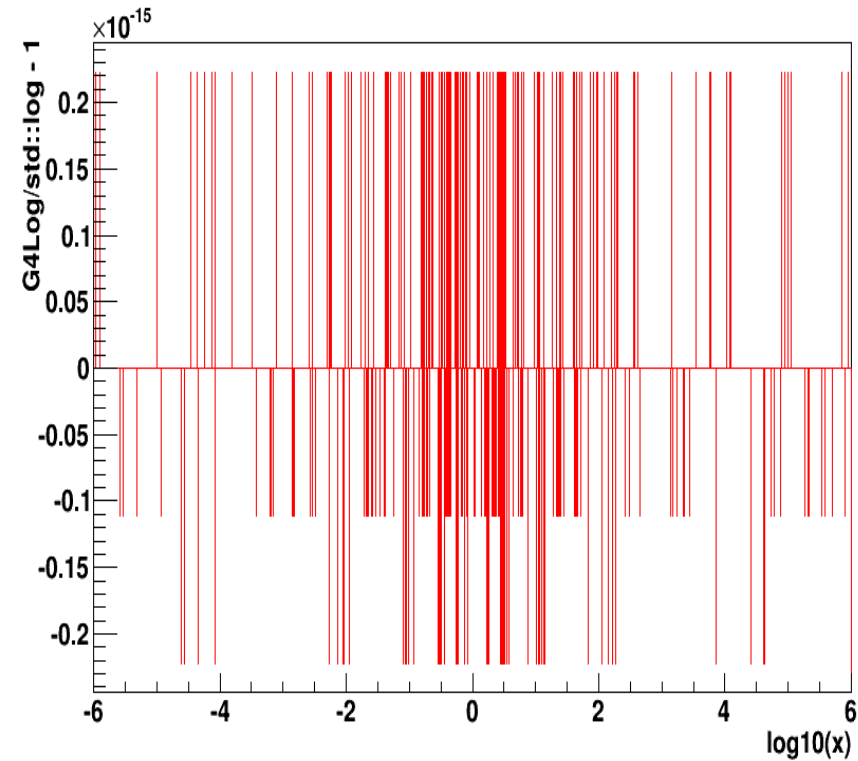


G4Log and G4Exp



- ∞ Danilo Piparo, Thomas Hauth, Vincenzo Innocente developed VDT mathematical library
 - ∞ Alternative to cmath
 - ∞ May be preloaded and substitute standard library
 - ∞ This is not very convenient from management point of view
- ∞ In Geant4 9.6ref09 two new classes are added G4Log and G4Exp
 - ∞ These classes are extracted by me from VDT
 - ∞ Were adapted to Geant4 platforms by Gabriele Cosmo

Accuracy of G4Log and G4Exp



CPU performance



	Std	G4 VDT	G4Pow
Log	8.97	4.91	5.19
Exp	13.93	1.95	1.34
$A^{1/3}$	20.46	7.03	0.77
$Z^{1/3}$	-	-	0.01

**Random number generator was used to select arguments of math functions
«background time» was subtracted**

Data Classes Evolution



- ❧ Main data classes:
 - ❧ **G4PhysicsVector** - was there from the beginning
 - ❧ **G4Physics2DVector** - introduced for SeltzerBerger model for g4 9.5
 - ❧ Now also used by muon models
 - ❧ **G4ElementData** introduced for Geant4 9.6 to keep atomic data
 - ❧ Livermore photo-electric
 - ❧ Muon models
 - ❧ NeutronXS
- ❧ For MT prototype these classes were developed as «splitted» - cache was thread local, mail class shared
- ❧ For 10.0beta and just after a design iteration was done
 - ❧ Splitted classes provide too many problems for MT
 - ❧ Design was not elegant
 - ❧ Now these classes are read-only in run time, no cache
 - ❧ No CPU penalty when cache sub-classes were removed
 - ❧ User code if needed may have tread local cache implementation
 - ❧ This is not needed in many Geant4 cases

Recent Updates



- ⌘ `G4PhysicsVector::Value(e)` is one of the most frequently called methods seen in the top of all profiling results
 - ⌘ It calls bin location method
 - ⌘ In EM usually logarithmic vector is used
 - ⌘ `Std::log` was substituted by `G4Pow::logX()`
 - ⌘ A new method `G4PhysicsVector::Value(e, idx)` was introduced as an alternative
 - ⌘ This method allows user code to have cache avoiding call to bin location
 - ⌘ A new method `G4PhysicsVector::SampleLinearX()` was introduced for cumulative functions providing linear sampling of argument according to the distribution
 - ⌘ This allows to remove duplicated code in different Geant4 classes
- ⌘ The same updates were introduced in `G4Physics2DVector`

Migration to MT



- ⌘ Having read-only physics vectors is very convenient for MT mode
 - ⌘ Before this migration there were difficulties in debugging of Geant4 in MT mode
- ⌘ All classes based its internal data on G4ElementData structures were easily migrated to MT providing sharing these data between threads

Summary and «to do»



- ⌘ CPU effect of VDT and G4Pow math functions is very significant, so for 10.0 we need:
 - ⌘ migrate all sensitive code (cross sections first of all) to
 - ⌘ G4Log, G4Exp, G4Pow::A13, G4Pow::A23
 - ⌘ If there are math functions with integer arguments then migrate to
 - ⌘ G4Pow::Z13, G4Pow::Z23, G4Pow::logZ, G4Pow::factorial
- ⌘ Data structure classes redesign was an essential part of MT migration
 - ⌘ The next step is to make G4PhysicsVector be free of virtual methods