# Geant4: improving computing performance by removing redundant G4Log calls

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## Outline

**Geant4: improving computing performance by removing redundant G4Log calls**

1. Motivation

**Everything started with the `G4EmElementSelector`[1]:**

- for EM models, the `G4VEmModel` base class provides the possibility to (automatically)build a collection of `G4EmElementSelector`-s for each material cuts couple
- this collection can be used at run-time, to sample the target atom for the given interaction (in case of multi-element materials)
- each individual (i.e. for a given *model* given *material* cuts couple) `G4EmElementSelector` of the collection stores a table of discrete probabilities of having the given interaction on a given element of the material (i.e. $P(Z_i) = \Sigma_{Z_i}/\Sigma$) over a discrete energy grid: equally spaced in log energy scale
- the implementation of the table is a vector of `G4PhysicsLogVector` (as many as elements in the given material)
- at run-time, the target atom is sampled according to this discrete probability distribution: the probabilities are interpolated for the given primary energy
- however, **the energy bin index was re-computed for each possible target element during the interpolation: because selectors are individual log-vectors** (was fixed in `10.05`)

[1] see my presentation at the last collaboration meeting in Lund (Section 3. from slide #37 here)

## The issue was however more general:

- the above G4EmElementSelector problem, i.e. extensive use of the G4Log, was clearly shown by the profiling done as part of the new G4SeltzerBergerModel development[1]
- however, the origin of the issue was in the underlying G4PhysicsLogVector
- G4PhysicsLogVector is heavily used in Geant4 to store kinetic energy dependent data ($\mathrm{d}E/\mathrm{d}x$, $R$, $\Sigma_t$, $\Sigma_{Z_i}$, $\sigma$, etc.) in a discretised form and to obtain interpolated values at run-time
- at the interpolation, the logarithm of the actual kinetic energy value i.e. G4Log(E_k) needs to be known (for the computation of the abscissa bin index i such that $E_i \leq E_k < E_{i+1}$)
- the bin index is very often computed, i.e. G4Log(E_k) is evaluated, in spite of the fact that the last index used ilast is (often) cached and checked before the bin index computation
- on the same time, these G4PhysicsLogVectors are accessed at each simulation step to provide values needed to determine the actual physics step length: **individual table accesses with the same value of E_k results in redundant G4Log(E_k) computations**
- this is the main source of the significant run-time cost of the G4PhysicsVector::Value( G4double E_k, size_t& ilast) method that could have been observed for a long time

[1] see my presentation at the last collaboration meeting in Lund (Section 2. from slide #30 here)

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2 Solution

**To avoid redundant computations of `G4Log(E_k)`, the proposed [1] solution was applied:**

- to (1) store the logarithm of the kinetic energy whenever is already computed:

```
inline void G4DynamicParticle::SetKineticEnergy(G4double aEnergy)
{
  isLogEkinUpToDate = ( isLogEkinUpToDate && (theKineticEnergy == aEnergy) );
  theKineticEnergy = aEnergy;
}
```

```
inline G4double G4DynamicParticle::GetLogKineticEnergy() const
{
  if (!isLogEkinUpToDate) {
    theLogKineticEnergy = (theKineticEnergy > 0.) ?
                          G4Log(theKineticEnergy) : LOG_EKIN_MIN;
    isLogEkinUpToDate   = true;
  }
  return theLogKineticEnergy;
}
```

- and (2) propagate to the interpolation method i.e. introduce a new `G4PhysicsVector::Value( G4double E_k, G4double LogE_k, size_t& ilast)` method

```
G4double G4PhysicsVector::Value(G4double theEnergy, G4double theLogEnergy,
                                size_t& lastIdx) const
```

[1] see my presentation at the last collaboration meeting in Lund (Section 3. slide #40 here)

## Additional information:

- about 40 files have been modified over 5 categories to introduce and to make use of the new functionality
- the simulation results are not affected by the changes: results stay **numerically identical** before and after merging the corresponding changes
- the profiling results shown in the following slides were obtained by:
  - using `valgrind` with the `--tool=callgrind`
  - instrumentation only in the event-loop: `CALLGRIND_START_INSTRUMENTATION` and `CALLGRIND_STOP_INSTRUMENTATION` at the end/beginning of the `Begin-/EndOf RunAction` with the `--instr-atstart=no` (i.e. pure run-time contributions are measured)
  - `Geant4-10.05-ref02` refers to the `-ref02` master **before** while `Geant4-10.05-ref03` to the master **after** merging the corresponding changes
  - both versions of `Geant4` were build and used in `DEBUG` mode during the profiling to see all `inlined` methods (i.e. look only the call counters and do not give significance neither to the inclusive nor to the exclusive performance contributions)

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3 Results

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# 3 Results

## Electromagnetic component

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**10 [GeV] $e^-$ in Simplified Sampling Calorimeter**: 50 layers of 2.5 [mm] Pb and 5.7 [mm] liquid-Ar

`Geant4-10.05-ref02`:

| Incl. | Self | Called | Function |
|---|---|---|---|
| 9.48 | 0.67 | 40 680 456 | G4PhysicsVector::Value(double, unsigned long&) const |

[1] see my presentation at the last collaboration meeting in Lund (Section 3. slide #40 here)

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`Geant4-10.05-ref03`: with the new `Value(E_k, LogE_k, ilast)` interface method

| Incl. | Self | Called | Function |
|---|---|---|---|
| 5.01 | 0.52 | 30 353 168 | G4PhysicsVector::Value(double, double, unsigned long&) ... |
| 2.45 | 0.18 | 10 327 288 | G4PhysicsVector::Value(double, unsigned long&) const |

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**~25 % goes through the old** while **~75 % goes through the new interface**

`Geant4-10.05-ref03`: with the new `Value(E_k, LogE_k, ilast)` interface method

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| 5.01 | 0.52 | 30 353 168 | G4PhysicsVector::Value(double, double, unsigned long&) ... |
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| Incl. | Self | Called | Function |
|---|---|---|---|
| 6.57 | 1.95 | 57 714 780 | G4Log(double) |

`Geant4-10.05-ref03`: **~24 % reduction in run-time `G4Log`-calls for EM shower**[1]

| Incl. | Self | Called | Function |
|---|---|---|---|
| 5.01 | 0.52 | 30 353 168 | G4PhysicsVector::Value(double, double, unsigned long&) ... |
| 2.45 | 0.18 | 10 327 288 | G4PhysicsVector::Value(double, unsigned long&) const |

| Incl. | Self | Called | Function |
|---|---|---|---|
| 4.96 | 1.47 | 44 014 751 | G4Log(double) |

[1] see my presentation at the last collaboration meeting in Lund (Section 3. slide #40 here)

**Geant4: improving computing performance by removing redundant G4Log calls**

## 3 Results

### Including hadronic component

## Including hadronic component

**CMS simulation**: 100 random (particle, direction, energy $\in$ [1GeV − 100GeV]) events without field

Geant4-10.05-ref02:

| Incl. | Self | Called | Function |
|---|---|---|---|
| 9.97 | 0.68 | 320 702 629 | G4PhysicsVector::Value(double, unsigned long&) const |
| 7.35 | 0.25 | 222 889 366 | G4PhysicsVector::Value(double) const |

**An additional `Value(G4double E_k)` interface method:**

- that eventually calls the earlier `Value(G4double E_k, size_t& ilast)` interface method
- used mainly (~97%) by neutron XS (elastic, inelastic, xapture)
- do not benefit from cached last bin index used → `G4Log` is always recomputed !

```
inline
G4double G4PhysicsVector::Value(G4double theEnergy) const
{
  size_t idx=0;
  return Value(theEnergy, idx);
}
```

## Including hadronic component

**CMS simulation**: 100 random (particle, direction, energy ∈ [1GeV − 100GeV]) events without field

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| 9.97 | 0.68 | 320 702 629 | G4PhysicsVector::Value(double, unsigned long&) const |
| 7.35 | 0.25 | 222 889 366 | G4PhysicsVector::Value(double) const |

`Geant4-10.05-ref03`: with the new `Value(E_k, LogE_k, ilast)` interface method

| Incl. | Self | Called | Function |
|---|---|---|---|
| 5.42 | 0.69 | 304 046 692 | G4PhysicsVector::Value(double, double, unsigned long... |
| 0.69 | 0.04 | 16 655 937 | G4PhysicsVector::Value(double, unsigned long&) const |
| 0.29 | 0.00 | 4 275 138 | G4PhysicsVector::Value(double) const |

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**~98 % reduction in Value(G4double E_k) calls**

**~5 % goes through the old** while **~95 % goes through the new interface**

Geant4-10.05-ref03: with the new Value(E_k, LogE_k, ilast) interface method

| Incl. | Self | Called | Function |
|---|---|---|---|
| 5.42 | 0.69 | 304 046 692 | G4PhysicsVector::Value(double, double, unsigned long... |
| 0.69 | 0.04 | 16 655 937 | G4PhysicsVector::Value(double, unsigned long&) const |
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**CMS simulation**: 100 random (particle, direction, energy $\in$ [1GeV − 100GeV]) events without field

Geant4-10.05-ref02:

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| 9.97 | 0.68 | 320 702 629 | G4PhysicsVector::Value(double, unsigned long&) const |
| 7.35 | 0.25 | 222 889 366 | G4PhysicsVector::Value(double) const |

| Incl. | Self | Called | Function |
|---|---|---|---|
| 4.93 | 1.46 | 322 222 206 | G4Log(double) |

Geant4-10.05-ref03: ~62 % reduction in run-time G4Log-calls !!!

| Incl. | Self | Called | Function |
|---|---|---|---|
| 5.42 | 0.69 | 304 046 692 | G4PhysicsVector::Value(double, double, unsigned long... |
| 0.69 | 0.04 | 16 655 937 | G4PhysicsVector::Value(double, unsigned long&) const |
| 0.29 | 0.00 | 4 275 138 | G4PhysicsVector::Value(double) const |

| Incl. | Self | Called | Function |
|---|---|---|---|
| 1.94 | 0.58 | 124 351 365 | G4Log(double) |

## Geant4: improving computing performance by removing redundant G4Log calls

### 3 Results

Performance analysis

## Performance analysis

**Two architectures**:

- **AMD**: AMD Desktop (SLC 6.10 Carbon), 3.5 GHz AMD PRO A10-9700 R7 processor with 8 GB DDR4-2400 SDRAM memory and gcc 8.2.0 (sourced from /cvmfs/sft.cern.ch/lcg/... i.e. not local)
- **MacBook**: MacBook Pro (MacOS 10.13.2), 2.8 GHz Intel Core i7 processor with 16 GB 1600 MHz DDR3 memory using Apple LLVM v10.0.0 (clang-1000.10.44.4) (local)

**Two applications**:

**HadCalCMS (EM shower):**

- Application : simplified (Cu-lAr) sampling calorimeter simulation
- Field : constant (4 or $10^{-5}$ [T]) or zero magnetic field
- Events : 50 [GeV] $e^{-}$ with FTFP_BERT physics list
- Run : 200 Events

**fullCMS (combined EM-Hadronic shower):**

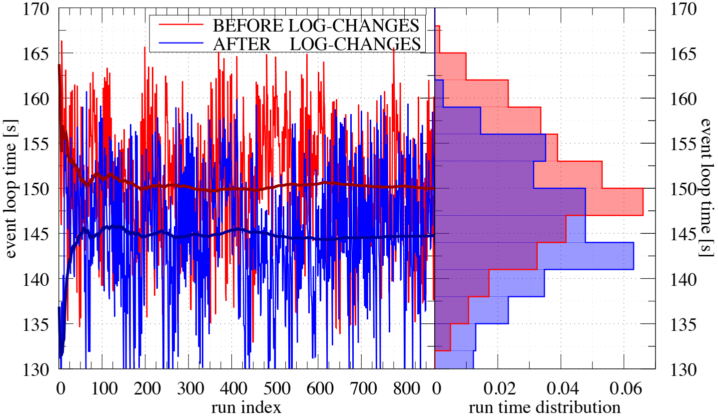
- Application : simulation application using the complete CMS detector
- Field : no field
- Events : random particle type, direction, energy with FTFP_BERT p. list
- Run : 100 Events

## Performance analysis

**NOTE:** not easy to obtain stable time measurement i.e. with small $\sigma$ (fullCMS on AMD): **INITIAL**

SHARED Geant4 + no-field: $\tilde{t} = 149.99, \tilde{\sigma} = 6.78$ v.s. $\tilde{t} = 144.8, \tilde{\sigma} = 7.24 \rightarrow$ -**3.46** %

3 Run-s per Execution and all Run-s are used

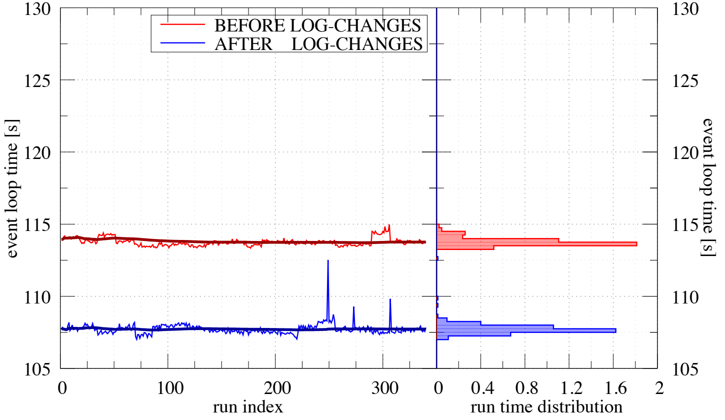


## Performance analysis

**NOTE:** not easy to obtain stable time measurement i.e. with small $\sigma$ (fullCMS on AMD): **FINAL**

STATIC Geant4 + no-field: $\tilde{t} = 113.75, \tilde{\sigma} = 0.26$ v.s. $\tilde{t} = 107.72, \tilde{\sigma} = 0.39 \rightarrow$ **-5.3** %

20 Run-s per Execution and the first 3 Run-s are excluded from each Execution



## Performance analysis

**The corresponding performance improvements**:

`fullCMS` **(combined EM-Hadronic shower)**:

- ~**8** % on my **MacBook Pro** (MacOS 10.13.2), 2.8 GHz Intel Core i7 processor with 16 GB 1600 MHz DDR3 memory using Apple LLVM version 10.0.0 (clang-1000.10.44.4) (**all local**)
- ~**5.3** % on my **AMD Desktop** (SLC 6.10 Carbon), 3.5 GHz AMD PRO A10-9700 R7 processor with 8 GB DDR4-2400 SDRAM memory using gcc 8.2.0 sourced from /cvmfs/sft.cern.ch/lcg/... (i.e. **not all local**)

`HadCalCMS` **(pure EM-shower)**:

- ~**2.3-4.2** % on my **MacBook Pro** (MacOS 10.13.2), 2.8 GHz Intel Core i7 processor with 16 GB 1600 MHz DDR3 memory using Apple LLVM version 10.0.0 (clang-1000.10.44.4) (**all local**)
- ~**2.3** % on my **AMD Desktop** (SLC 6.10 Carbon), 3.5 GHz AMD PRO A10-9700 R7 processor with 8 GB DDR4-2400 SDRAM memory using gcc 8.2.0 sourced from /cvmfs/sft.cern.ch/lcg/... (i.e. **not all local**)

## Outline

**`Geant4`: improving computing performance by removing redundant `G4Log` calls**

4. **Further optimisations of the `G4PhysicsVector`**

**Beyond some possible micro-optimisations the following will be considered :**

- the `G4PhysicsVector` and its `Value` methods (even the new one) are still general:
  - covers all possible binning schemes (using `types` defined in `G4PhysicsVectorType`)
  - calling the `Value` method will call `FindBin` (after some checks)
  - `FindBin` will call `FindBinLocation` (after some checks)
  - that will eventually determine the lower bin index depending on the vector `type`
- however, when we use the new `Value(E_k, LogE_k, ilast)` method we know that the `type` is `T_G4PhysicsLogVector` (general = this method works even if the type is not `LogVector`)
- `LogVector` is the dominant `type` (see the `callgrind` results: EM - **75** %, EM-Hadronic - **95**%)
- make use of the `LogVector-type` information especially because its importance:
  - introduce a `G4PhysicsVector::LogVectorValue(E_k, LogE_k)` method
  - fully specialised for `T_G4PhysicsLogVector type`
  - simplifications(skips some checks: on the `type`, on the `ilast`) and streamlining
- results in an even more optimised usage of the `G4PhysicsVector` at run-time

# Outline

**Geant4: improving computing performance by removing redundant G4Log calls**

5 Conclusion

**A significant number of redundant G4Log calls have been eliminated:**

- by introducing functionality to store/retrieve (in `G4DynamicParticle`) and re-use the already computed `G4Log(E_k)` value
- ~**24-62** % of the run time `G4Log` calls are eliminated by making use of the new functionality in the EM and Hadronic (neutornXS) physics
- it gives measurable run-time improvement of ~**2-8** % depending on the application, configuration and architecture
- a new interpolation method, specialised for **`LogVector-type`** will be introduced: **`G4PhysicsVector:LogVectorValue(E_k, LogE_k)`**
- this will optimise even further the usage of the **`G4PhysicsVector`** at run-time and eliminate further fraction of its significant cost