Performance profiling of Experiments' Geant4 Simulations
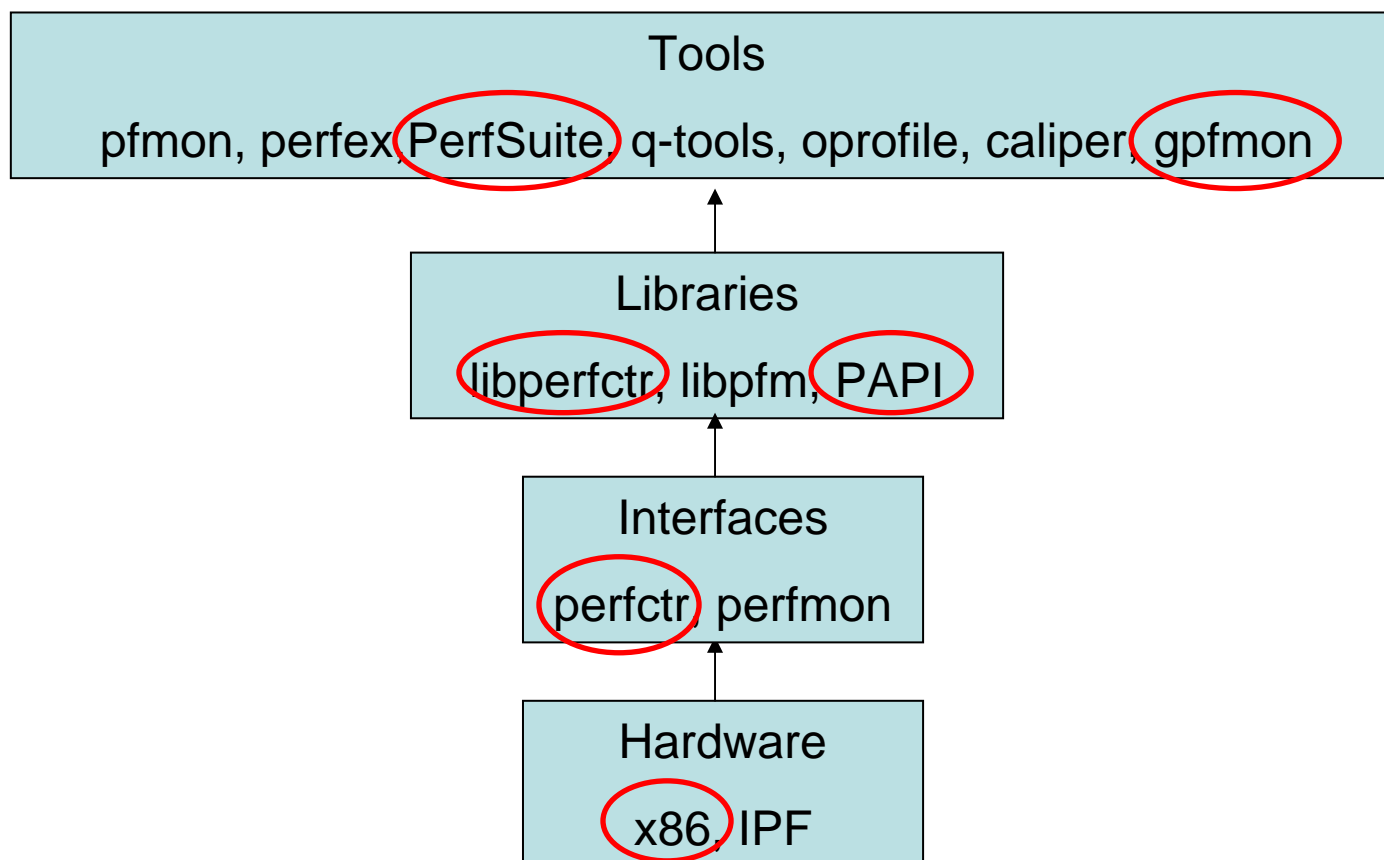
Geant4 Collaboration Workshop

14th October, Lisbon

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Introduction to Performance Profiling

- **Goal**
  - analysis of the behavior of a program while running
    - e.g. execution time, time spent per function, call graph
- **Software Instrumentation**
  - code snippets to collect required data
    - source (manual, gcc -pg)
    - binary (offline, online)
      - ✖ high overhead
- **Hardware approach**
  - special on-chip hardware of modern CPU
    - direct access to CPU resources (number of cycles, integer and floating point, instructions, branch prediction and miss-prediction, cache misses etc
    - event detectors, counters, Xeon (44,18)
    - ✓ less overhead
- **Hybrid solution**
  - both: instrumentation and hardware solutions

Tools

pfmon, perfex, PerfSuite, q-tools, oprofile, caliper, gpfmon

Libraries

libperfctr, libpfm, PAPI

Interfaces

perfctr, perfmon

Hardware

x86, IPF

- **Measurements on Xeon**
  - ✓ counting/sampling/profiling
  - ✓ user/kernel domain
  - ✓ per process/system-wide
  - ✓ counter multiplexing
  - ✓ kernel 2.4 & 2.6
  - ✗ number of function calls
    - ✓ we work on it, will be available soon
  - ✗ call graph
    - ✓ collaboration with interface developer in order to take advantage of hardware support

- http://perfsuite.ncsa.uiuc.edu (psrun, psprocess ...)
  - Open source collection of tools, utilities and libraries for software performance analysis
    - ✓ basic counting
    - ✓ sampling
    - ✓ user metrics
    - ✗ no system-wide mode
    - ✓ user/kernel domain
    - ✓ 2.4 & 2.6 kernel
    - ✓ profiling support
    - ✗ flat profile – neither number of function calls nor call graph

PerfSuite - challenges

- Does not work with python scripts running from command line

- unpredictable behavior on AFS (Andrew File System)

- a problem with resolving function names
  - unknown functions with static libraries
  - a huge problem with shared libraries
    - in order to monitor successfully, PerfSuite has to know all of them in advance
      - LD_PRELOAD variable – a big challange - how to select interesting libraries from 400+ without causing dependence error?
      - use other tools to have another look

PerfSuite & LD_PRELOAD

```
Profile Information
================================================
Class           : PAPI
Event           : PAPI_TOT_CYC (Total cycles)
Period          : 50000
Samples         : 719
Domain          : user
Run Time        : 17.52 (seconds)
Min Self %      : (all)
Module Summary
--------------------------------------------------
Samples  Self %  Total %  Module
  376   52.29%  52.29%  /usr/bin/python
  178   24.76%  77.05%  /lib/ld-2.3.2.so
  159   22.11%  99.17%  /lib/tls/libc-2.3.2.so
    4    0.56%  99.72%  /lib/tls/libpthread-0.60.so
    1    0.14%  99.86%  /lib/libdl-2.3.2.so
    1    0.14% 100.00%  /lib/libutil-2.3.2.so
Function Summary
--------------------------------------------------
Samples  Self %  Total %  Function
  376   52.29%  52.29%  ??
  110   15.30%  67.59%  do_lookup_versioned
   40    5.56%  73.16%  _int_malloc
   31    4.31%  77.47%  strcmp
   22    3.06%  80.53%  _dl_lookup_versioned_symbol
   19    2.64%  83.17%  memcpy
   16    2.23%  85.40%  __libc_malloc
   11    1.53%  86.93%  free
    7    0.97%  87.90%  _int_free
    7    0.97%  88.87%  strlen
    6    0.83%  89.71%  memset
    6    0.83%  90.54%  do_lookup
    5    0.70%  91.24%  malloc_consolidate
    5    0.70%  91.93%  __mempcpy
    4    0.56%  92.49%  __i686.get_pc_thunk.bx
    3    0.42%  92.91%  strerror_r
    3    0.42%  93.32%  mremap_chunk
    3    0.42%  93.74%  _int_realloc
    2    0.28%  94.02%  .L969
    2    0.28%  94.30%  realloc
    2    0.28%  94.58%  mallopt
```

```
Profile Information
================================================
Class           : PAPI
Event           : PAPI_TOT_CYC (Total cycles)
Period          : 50000
Samples         : 721514
Domain          : user
Run Time        : 17.60 (seconds)
Min Self %      : (all)
Module Summary
--------------------------------------------------
Samples   Self %  Total %  Module
 465515  64.52%  64.52%  /afs/cern.ch/user/o/oplaatl3/testdll/libhello2.so.1
 255433  35.40%  99.92%  /afs/cern.ch/user/o/oplaatl3/testdll/libhello1.so.1
    391   0.05%  99.98%  /usr/bin/python
    145   0.02% 100.00%  /lib/tls/libc-2.3.2.so
     26   0.00% 100.00%  /lib/ld-2.3.2.so
      4   0.00% 100.00%  /lib/tls/libpthread-0.60.so
Function Summary
--------------------------------------------------
Samples   Self %  Total %  Function
 255433  35.40%  35.40%  hello(int*)
 254920  35.33%  70.73%  sum(int*)
 210595  29.19%  99.92%  count(int*, int)
    392   0.05%  99.98%  ??
     36   0.00%  99.98%  _int_malloc
     22   0.00%  99.98%  memcpy
     13   0.00%  99.99%  __libc_malloc
     11   0.00%  99.99%  free
     10   0.00%  99.99%  do_lookup_versioned
      7   0.00%  99.99%  strcmp
      6   0.00%  99.99%  __open_nocancel
      5   0.00%  99.99%  _int_free
      4   0.00%  99.99%  memset
      4   0.00%  99.99%  malloc_consolidate
```

- there is no tool which meets our requirements in the domain of system-wide monitoring (counting, sampling)
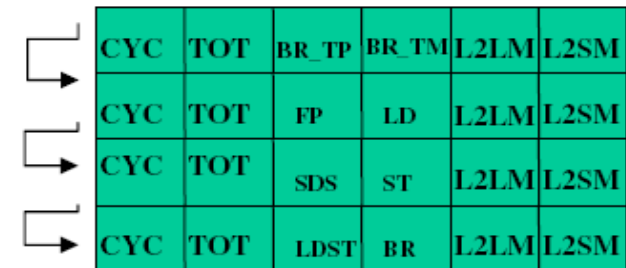- we decided to develop our own tool
  - gpfmon
    - uses perfctr interface and library
    - user/kernel domain
    - per single or total CPU
   - ✓ enables multiplexing
      - 4 even sets
        - cpu cycles, instructions completed, branches taken predicted and mispredicted, L2 load and store missed, FP, scalar, load and stores instructions
   - we miss average 2% samples, apart from L2 store missed – 92%

CYC	TOT	BR_TP	BR_TM	L2LM	L2SM
CYC	TOT	FP	LD	L2LM	L2SM
CYC	TOT	SDS	ST	L2LM	L2SM
CYC	TOT	LDST	BR	L2LM	L2SM

gpfmon sample results

- **Geant4 Atlas simulation**
  - IPC - 0.34
  - FP - 18%
  - LD+ST - 63% (7% LD caused L2 cache miss)
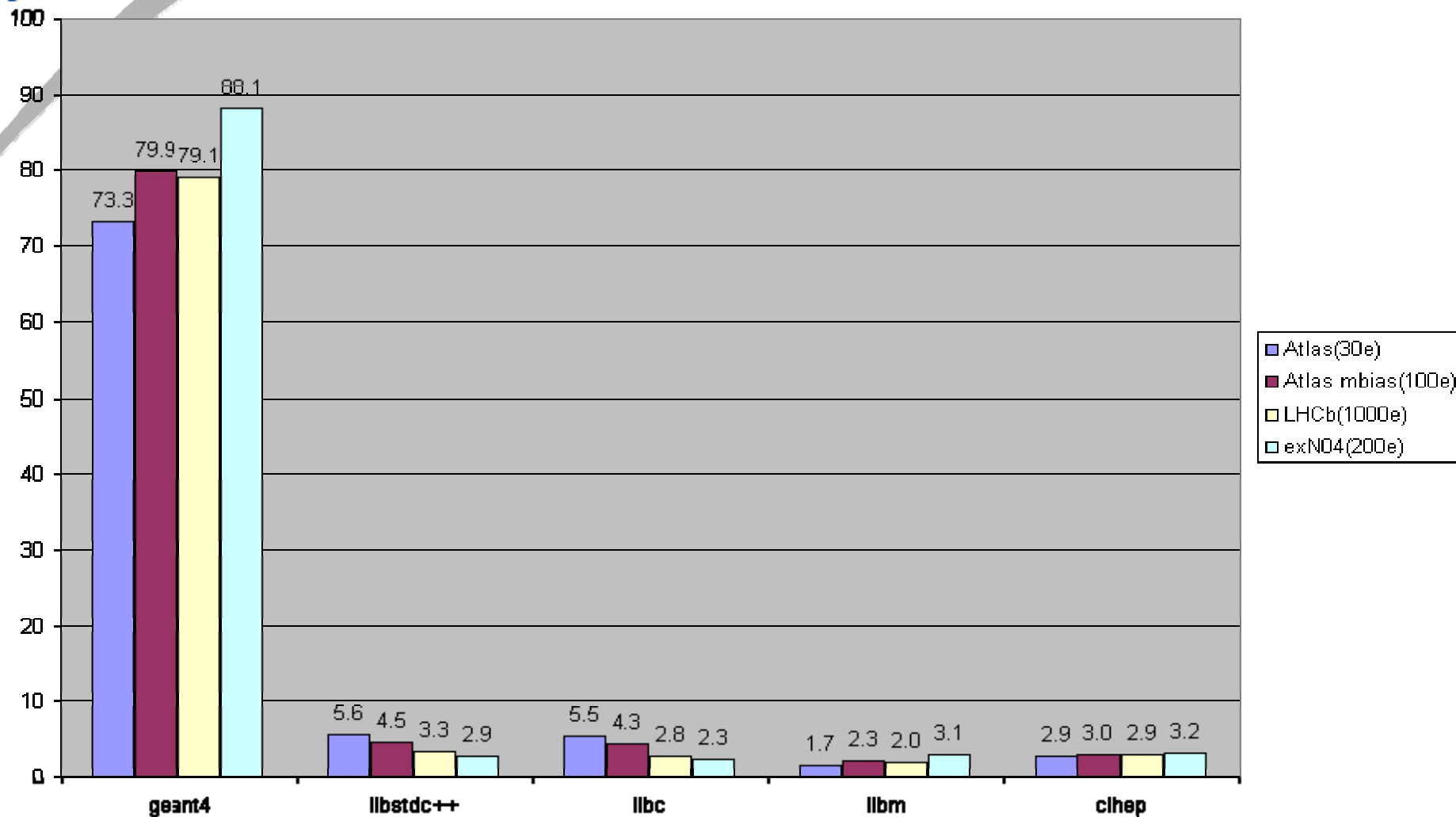 - Branches - 10%, ratio taken predicted/mispredicted=36

Total instructions/cycle
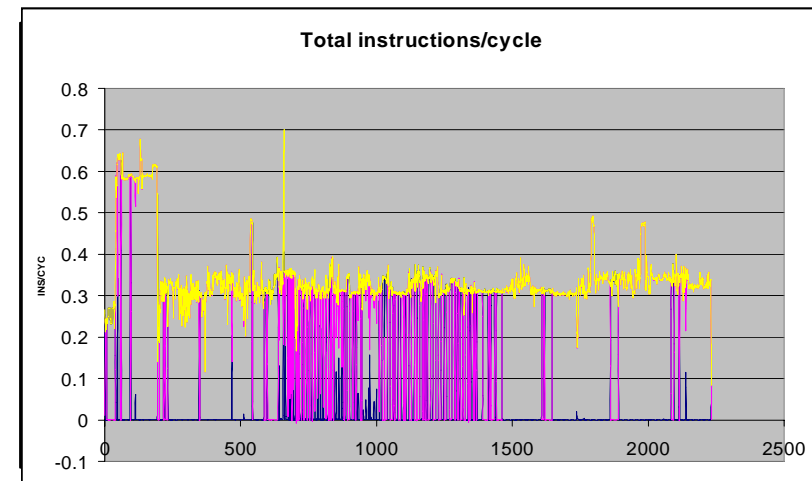
- **Atlas simulation**
  - full events (30), minimum-bias (100)

- **LHCb simulation**
  - 1000 events

- **Geant4 examples**
  - TestEm3
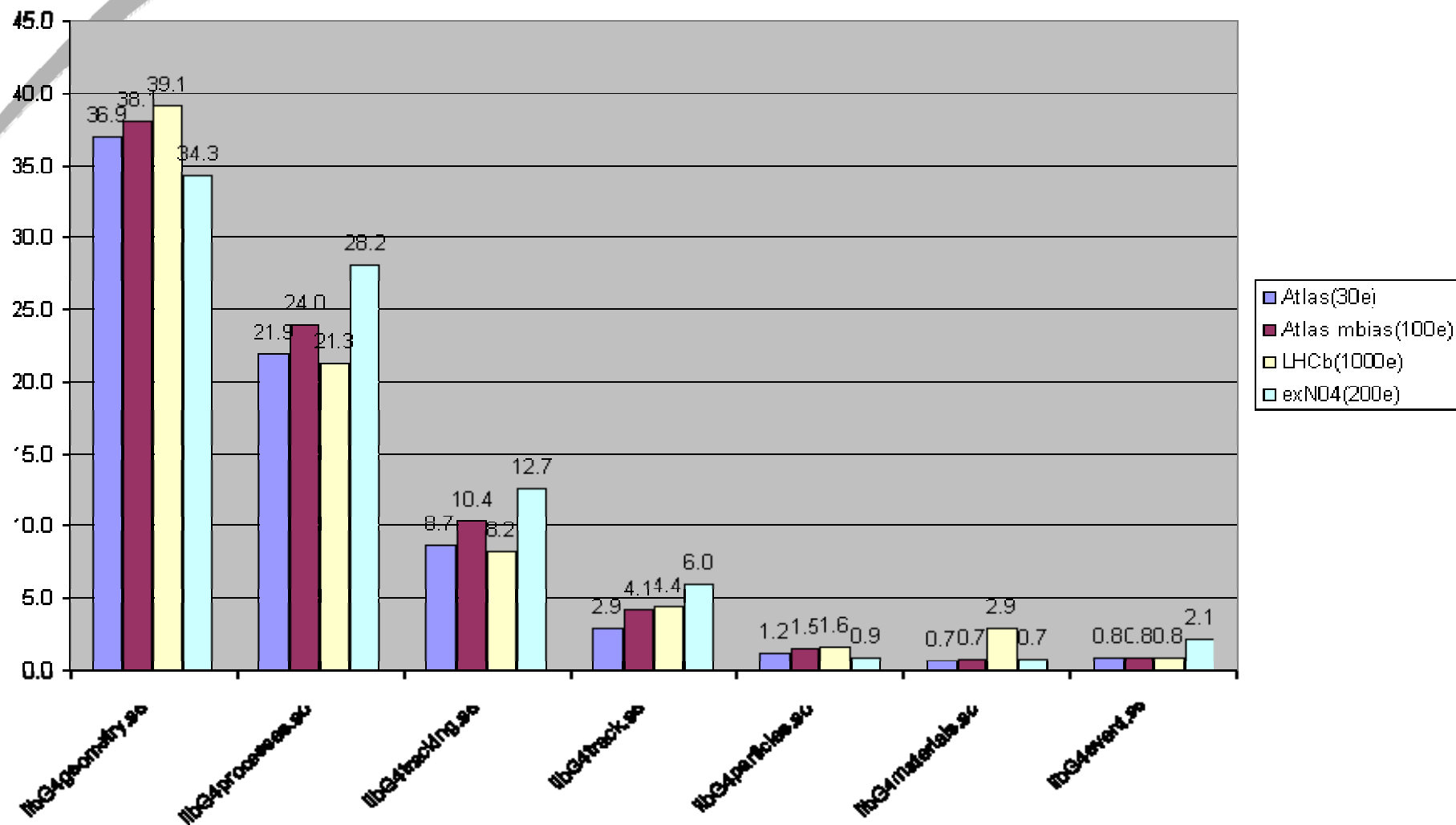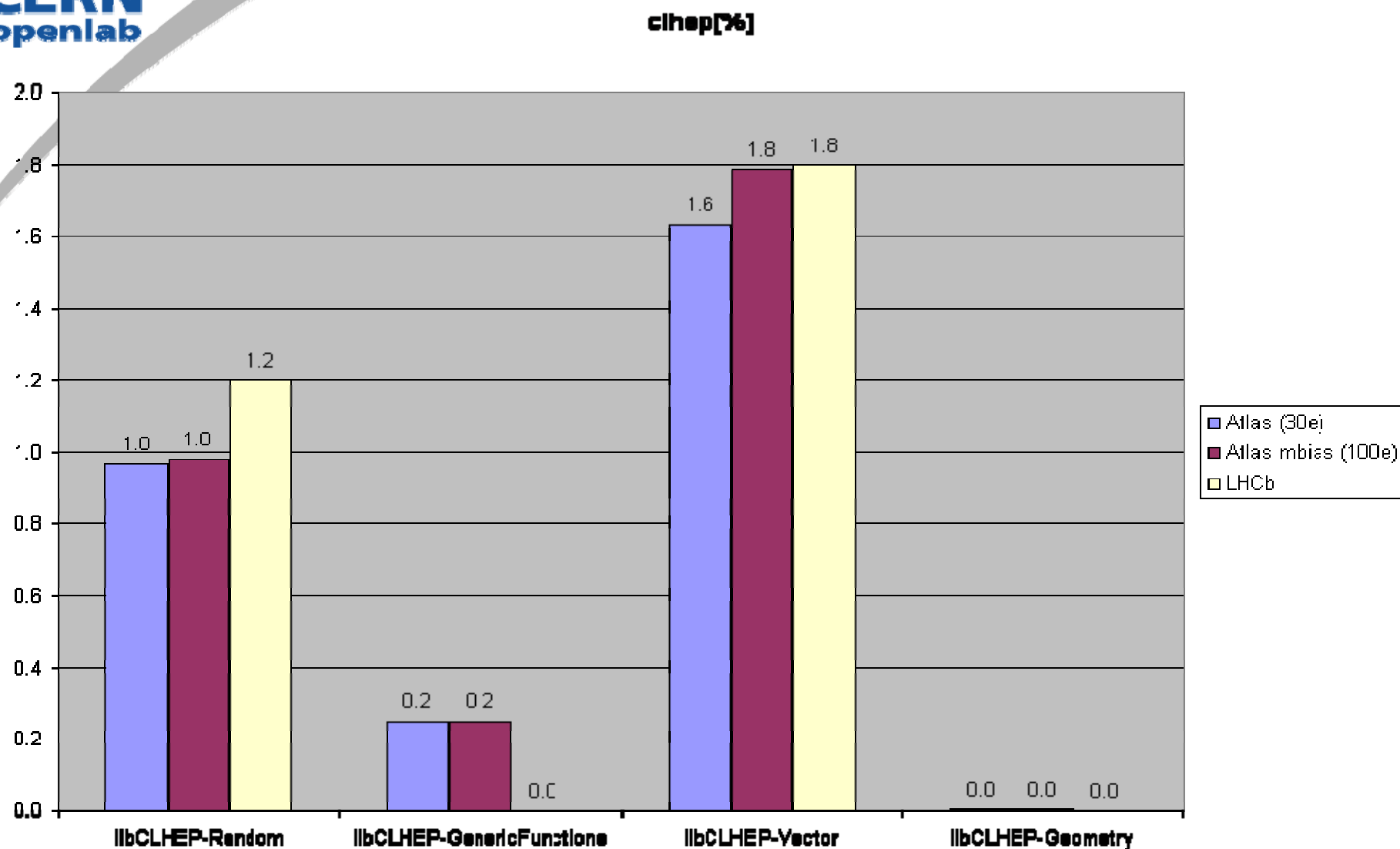 - example04
  - calorimeter regression test

- **Xeon 32bit mode**
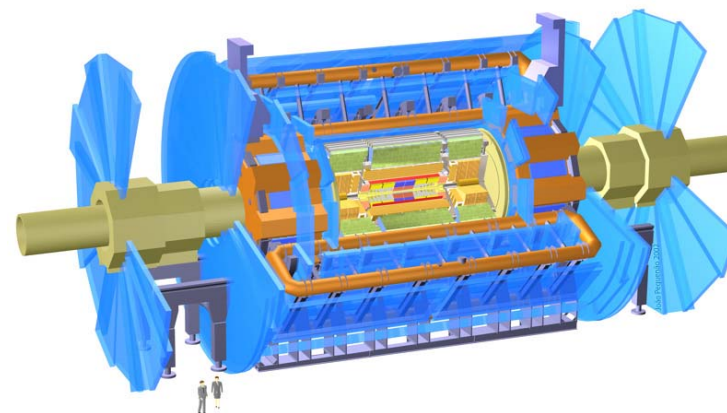
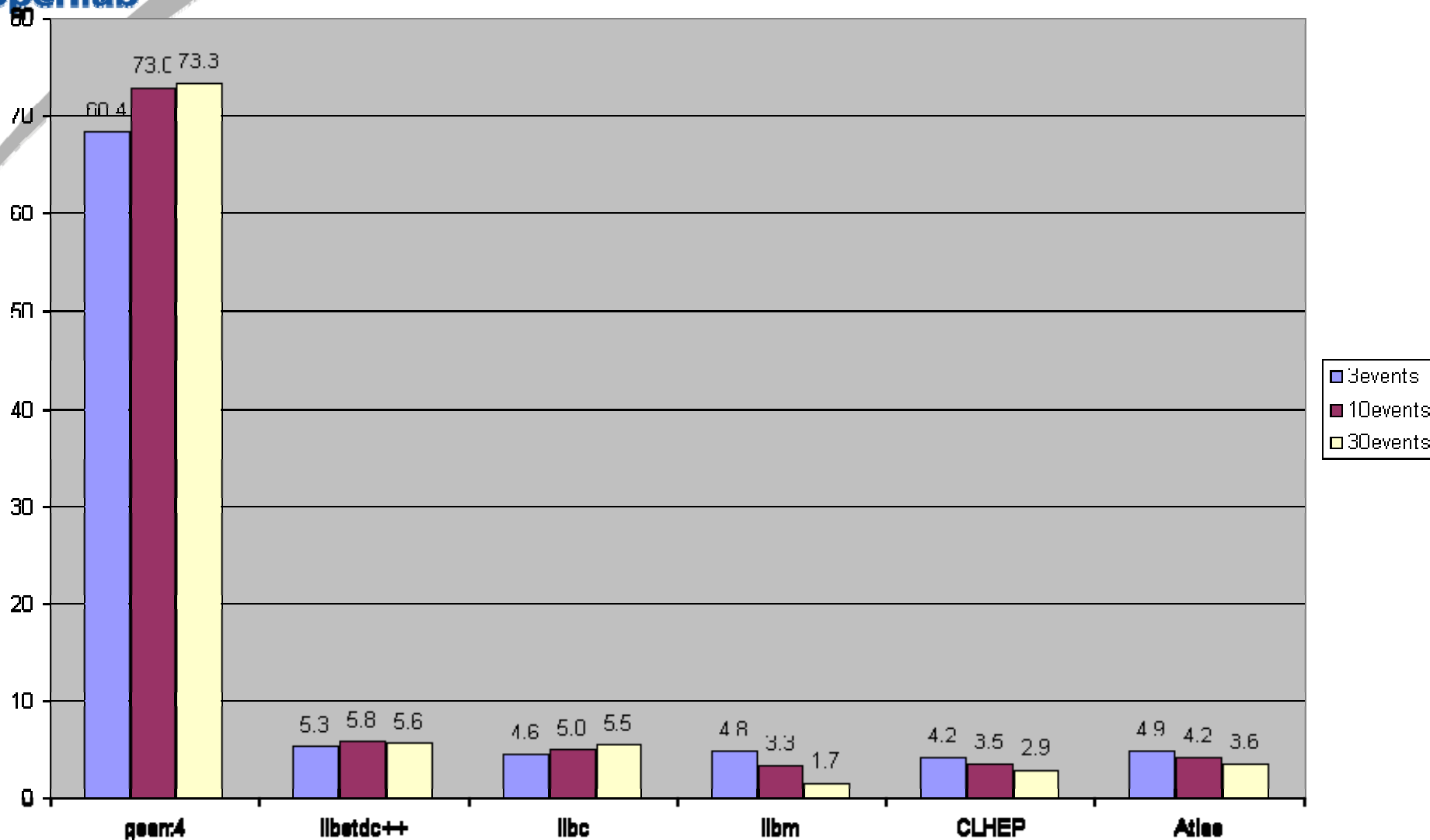- **Simulations**
    - Atlas
    - LHCb
- **Geant4 example N04**

Libraries[%]

geant4 libs[%]

clhep[%]

- **Atlas simulations**

Atlas Simulation[%]

Atlas - geant4 libraries[%]

Function Summary
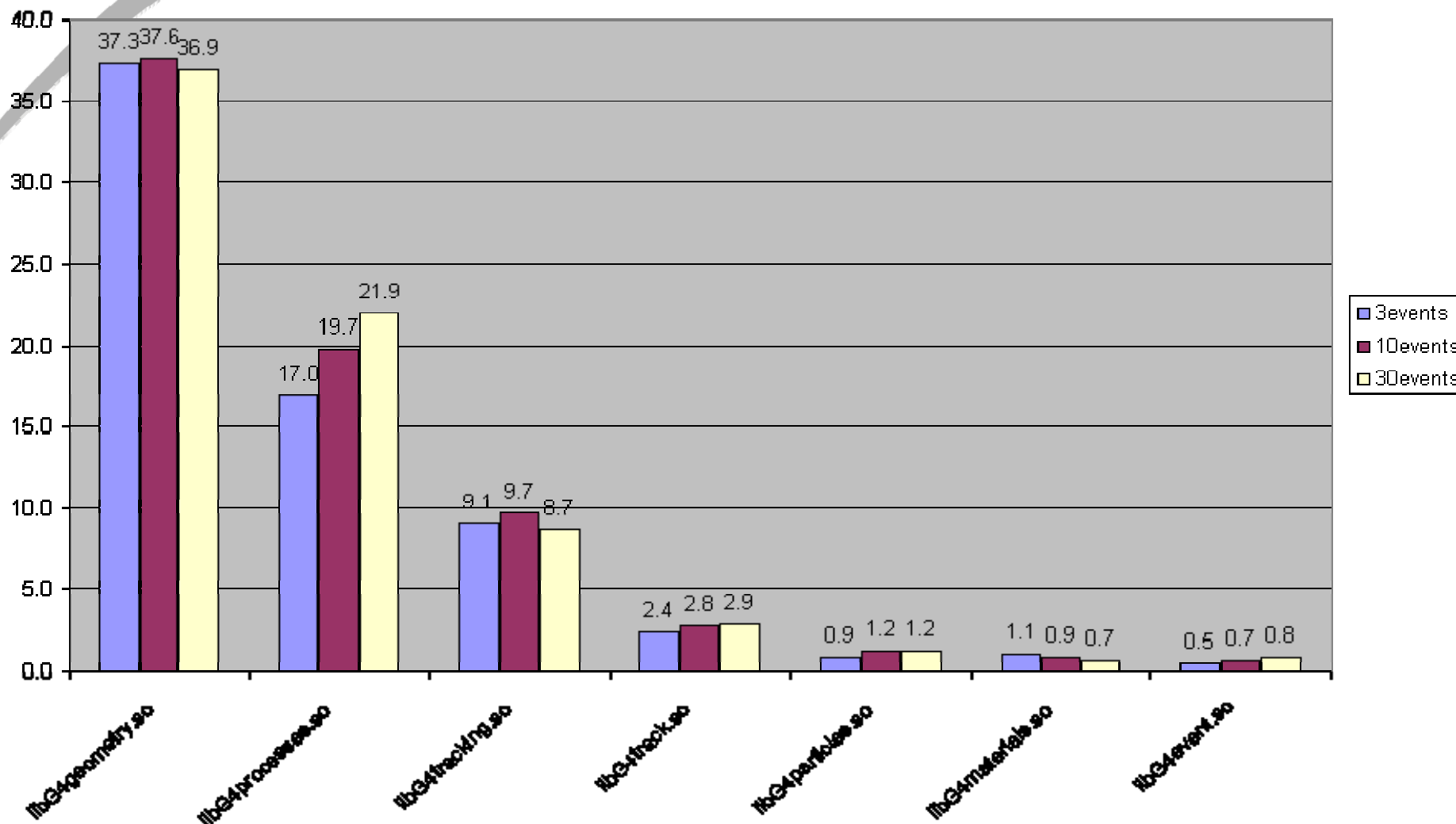
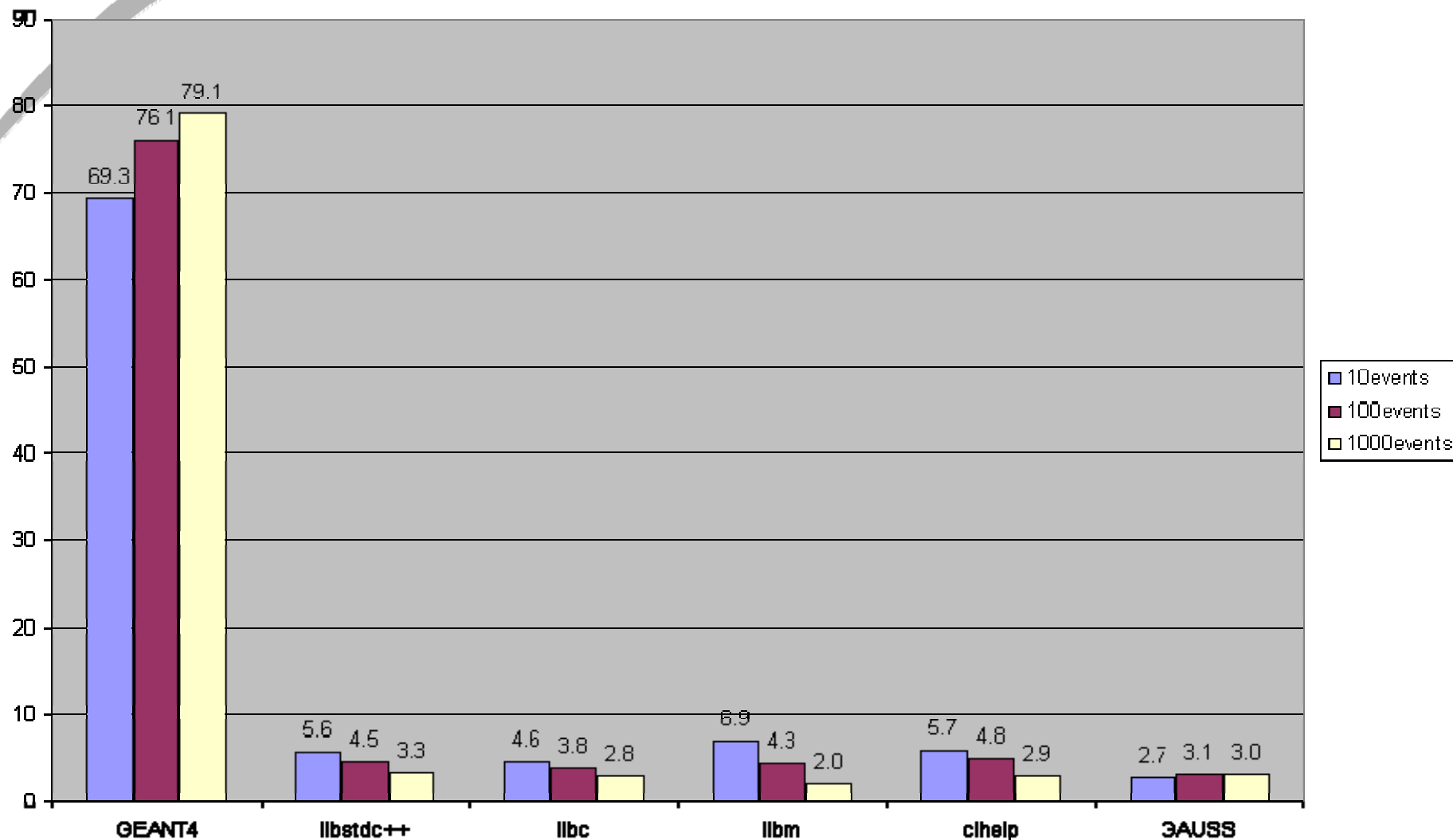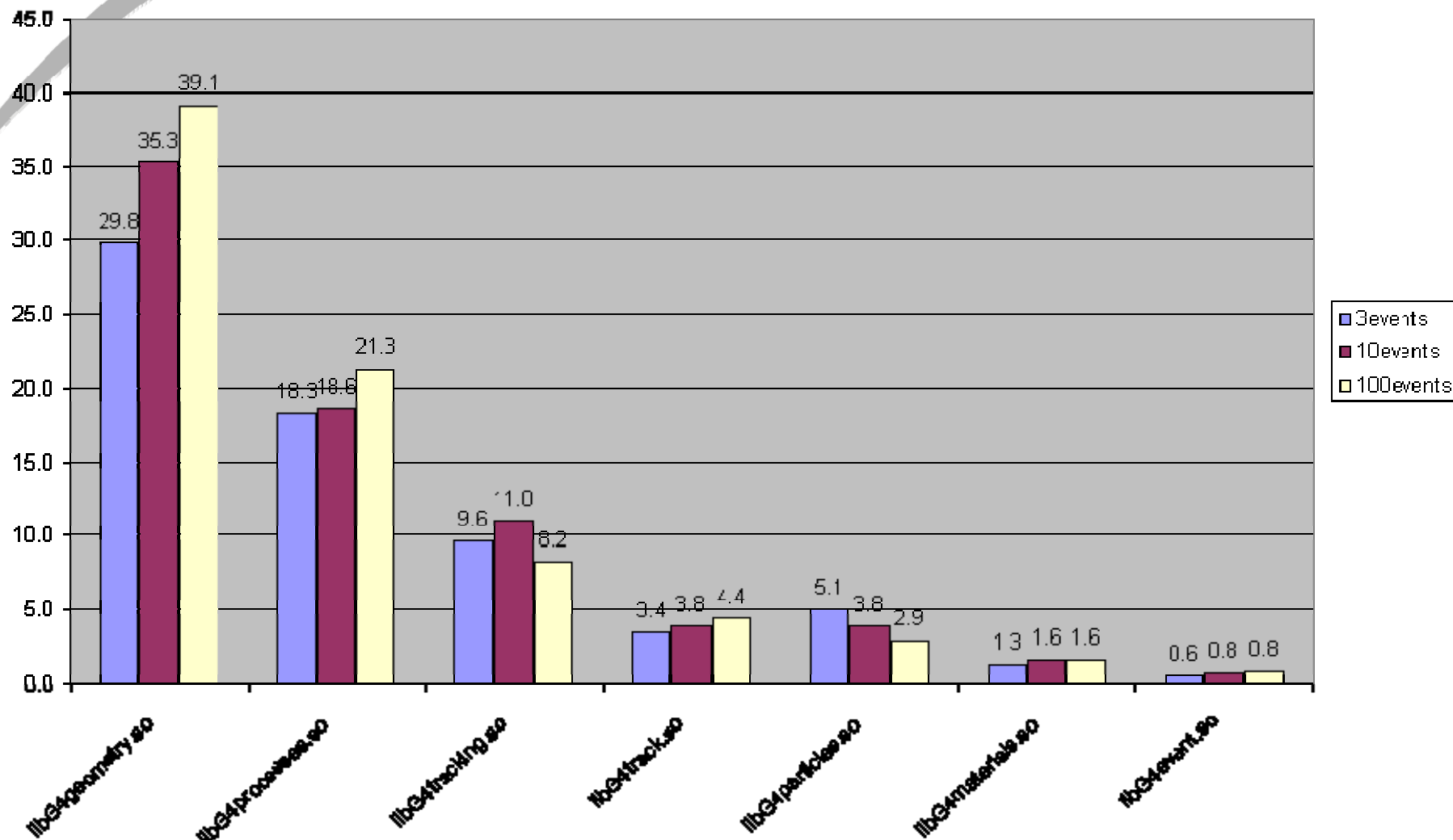| Samples	Self %	Total %	Function
30728046	**7.82%**	**7.82%**	**??**
7320624	1.86%	9.68%	G4Transportation::AlongStepGetPhysicalInteractionLength()
6689448	1.70%	11.38%	G4VoxelNavigation::ComputeStep()
5873290	1.49%	12.87%	G4Navigator::ComputeStep()
5490913	1.40%	14.27%	G4PolyconeSide::Intersect()
5278498	1.34%	15.61%	G4SteppingManager::Stepping()
5050076	1.28%	16.90%	G4PropagatorInField::ComputeStep()
4919562	1.25%	18.15%	G4Navigator::LocateGlobalPointAndSetup()
4503773	1.15%	19.30%	G4PolyconeSide::DistanceAway()
4366559	1.11%	20.41%	G4IntersectingCone::LineHitsCone1()
4295632	1.09%	21.50%	G4VoxelNavigation::LocateNextVoxel()
4199824	1.07%	22.57%	G4SteppingManager::DefinePhysicalStepLength()
4033883	1.03%	23.59%	G4MultipleScattering52::GetContinuousStepLimit()
3938509	1.00%	24.60%	G4SteppingManager::InvokePSDIP()
3912491	1.00%	25.59%	G4MultipleScattering52::PostStepDoIt()
3766114	0.96%	26.55%	G4ClassicalRK4::DumbStepper()
3722683	0.95%	27.50%	G4SteppingManager::InvokeAlongStepDoItProcs()
3620741	0.92%	28.42%	_int_malloc
3620692	0.92%	29.34%	G4Navigator::LocateGlobalPointAndUpdateTouchableHandle()
3604007	0.92%	30.25%	LArWheelCalculator::DistanceToTheNeutralFibre()
3598039	0.92%	31.17%	vfprintf
3581444	0.91%	32.08%	G4UniversalFluctuation::SampleFluctuations()
3259393	0.83%	32.91%	G4ElectroNuclearCrossSection::GetCrossSection()
3127408	0.80%	33.71%	G4PolyconeSide::PointOnCone()
2872853	0.73%	34.44%	G4NavigationLevelRep::G4NavigationLevelRep()
2833732	0.72%	35.16%	G4Transportation::PostStepDoIt()
2737712	0.70%	35.85%	G4ChordFinder::FindNextChord()
2733244	0.70%	36.55%	G4Tubs::DistanceToIn()
2721568	0.69%	37.24%	G4VEnergyLossProcess::AlongStepDoIt()
2654097	0.68%	37.92%	G4MagErrorStepper::Stepper()
2610649	0.66%	38.58%	G4ParticleChangeForTransport::UpdateStepForAlongStep()
2550219	0.65%	39.23%	G4SandiaTable::GetSandiaCofPerAtom()
2540628	0.65%	39.88%	G4PhotoNuclearCrossSection::GetCrossSection()
2413526	0.61%	40.49%	G4Transportation::AlongStepDoIt()
2407946	0.61%	41.10%	CLHEP::HepJamesRandom::flat()
2396557	0.61%	41.71%	G4PolyPhiFace::Intersect()
2390632	0.61%	42.32%	G4HadronCrossSections::CalcScatteringCrossSections()
2343439	0.60%	42.92%	G4MagInt_Driver::QuickAdvance()
2277101	0.58%	43.50%	CLHEP::HepRotation::rotateAxes()
2244256	0.57%	44.07%	G4PhysicsVector::GetValue()
2242211	0.57%	44.64%	G4SteppingManager::SetInitialStep()
2228671	0.57%	45.20%	G4Tubs::Inside()
2171964	0.55%	45.76%	G4NormalNavigation::ComputeStep()
2132567	0.54%	46.30%	G4VEmProcess::GetMeanFreePath()
2083184	0.53%	46.83%	G4VoxelNavigation::LevelLocate()
2067235	0.53%	47.35%	G4VoxelNavigation::ComputeVoxelSafety()
1978418	0.50%	47.86%	G4VoxelNavigation::VoxelLocate()
1944091	0.49%	48.35%	G4PropagatorInField::IntersectChord()
1892005	0.48%	48.83%	G4eBremsstrahlungModel::SampleSecondaries()
1889364	0.48%	49.31%	G4PolyconeSide::Inside()
1875195	0.48%	49.79%	G4PolyconeSide::Distance()
1853968	0.47%	50.26%	G4AffineTransform::G4AffineTransform()
1842997	0.47%	50.73%	G4EnclosingCylinder::MustBeOutside()
1841307	0.47%	51.20%	G4StepPoint::operator=()
1805522	0.46%	51.66%	G4ParticleChange::CheckIt()
1793612	0.46%	52.12%	G4VCSGfaceted::DistanceToOut()
1772012	0.45%	52.57%	G4TrackingManager::ProcessOneTrack()
1731569	0.44%	53.01%	G4HadronicProcess::GetMeanFreePath()
1631892	0.42%	53.42%	G4MagInt_Driver::AccurateAdvance()
1612075	0.41%	53.83%	G4ChordFinder::AdvanceChordLimited()
1546908	0.39%	54.23%	std::vector<G4VTrajectoryPoint*, std::allocator<G4VTrajectoryPoint*> >::_M_insert_aux()
1504737	0.38%	54.61%	G4VContinuousDiscreteProcess::PostStepGetPhysicalInteractionLength()
1471951	0.37%	54.98%	G4VEnergyLossProcess::GetMeanFreePath()
1456046	0.37%	55.35%	_int_free
1449124	0.37%	55.72%	G4VCSGfaceted::DistanceToIn()

- **LHCb simulation**

LHCb simulation[%]

Legend:
- 10events
- 100events
- 1000events

GEANT4: 69.3, 76.1, 79.1
libstdc++: 5.6, 4.5, 3.3
libc: 4.6, 3.8, 2.8
libm: 6.9, 4.3, 2.0
clhelp: 5.7, 4.8, 2.9
3AUSS: 2.7, 3.1, 3.0

LHCb simulation - geant4 libraries[%]

Function Summary

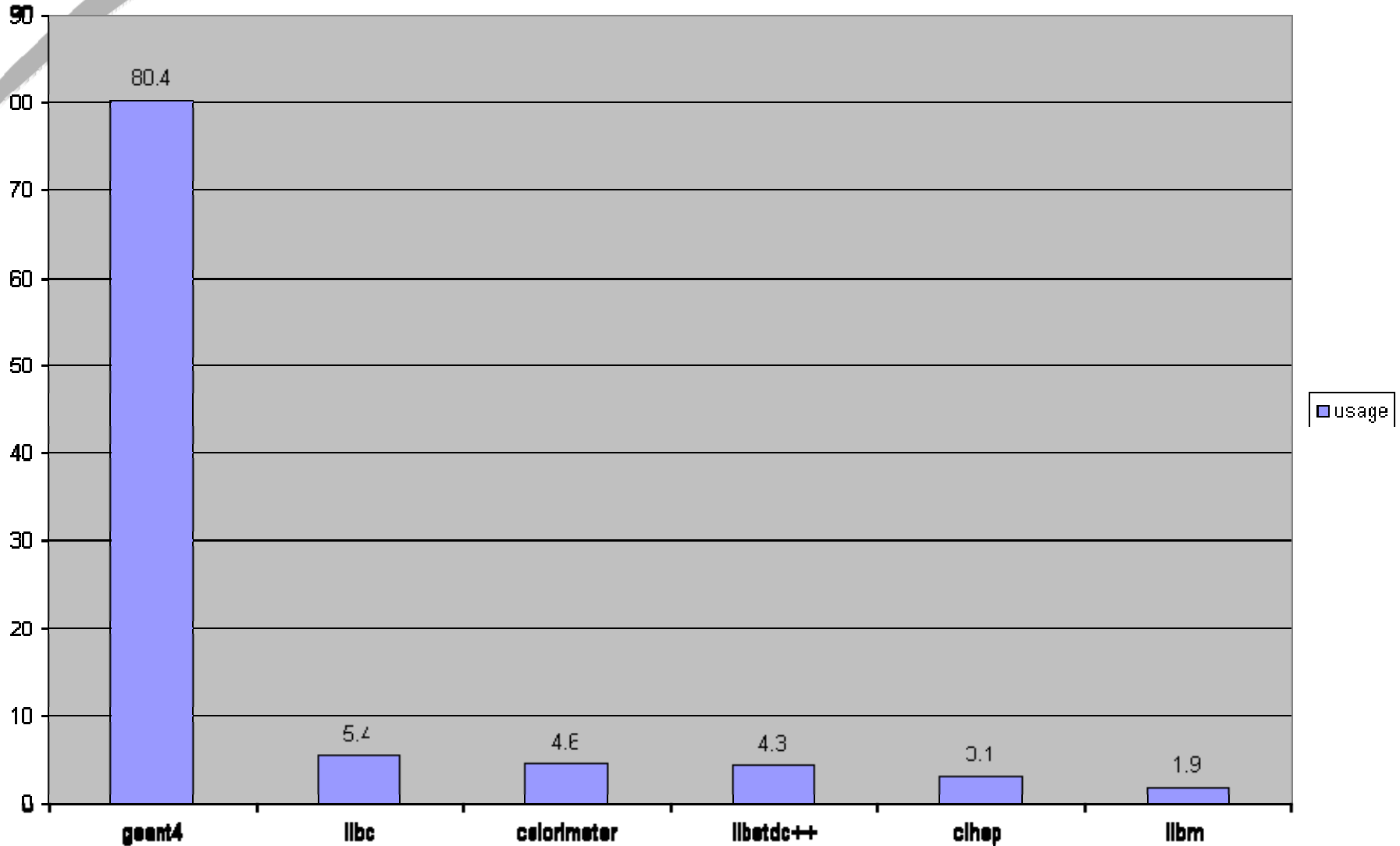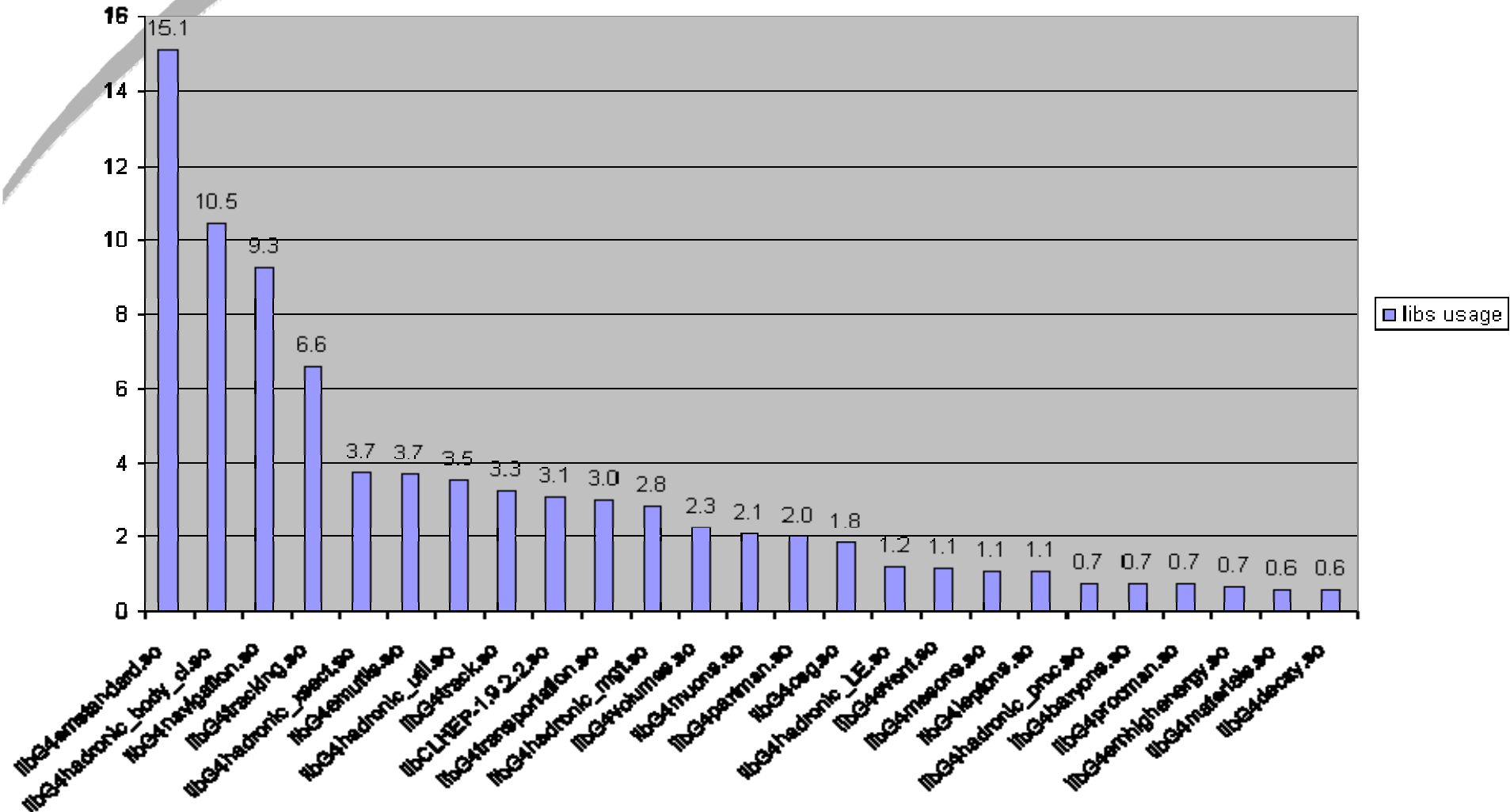| Samples	Self %	Total %	Function
18672274	4.49%	4.49%	??
8998975	2.16%	6.66%	G4VoxelNavigation::ComputeStep()
8123719	1.95%	8.61%	G4Transportation::AlongStepGetPhysicalInteractionLength()
7066865	1.70%	10.31%	G4VoxelNavigation::LocateNextVoxel()
6757801	1.63%	11.93%	G4Navigator::LocateGlobalPointAndSetup()
6716299	1.62%	13.55%	G4SteppingManager::InvokePSDIP()
6648670	1.60%	15.15%	G4Navigator::ComputeStep()
6237844	1.50%	16.65%	G4Navigator::LocateGlobalPointAndUpdateTouchableHandle()
5054291	1.22%	17.86%	G4NavigationLevelRep::G4NavigationLevelRep()
5053875	1.22%	19.08%	G4UniversalFluctuation::SampleFluctuations()
5015604	1.21%	20.29%	CLHEP::HepRotation::rotateAxes()
4970036	1.20%	21.48%	G4SteppingManager::InvokeAlongStepDoItProcs()
4894483	1.18%	22.66%	G4SteppingManager::Stepping()
4785378	1.15%	23.81%	G4HadronCrossSections::CalcScatteringCrossSections()
4564152	1.10%	24.91%	G4Box::DistanceToIn()
4262441	1.03%	25.93%	G4VoxelNavigation::LevelLocate()
3925503	0.94%	26.88%	_int_malloc
3818722	0.92%	27.80%	G4Transportation::AlongStepDoIt()
3662972	0.88%	28.68%	G4SteppingManager::SetInitialStep()
3480389	0.84%	29.51%	G4Transportation::PostStepDoIt()
3363825	0.81%	30.32%	G4MscModel::SampleCosineTheta()
3363389	0.81%	31.13%	G4PolyconeSide::DistanceAway()
3343872	0.80%	31.94%	G4VEnergyLossProcess::AlongStepDoIt()
3303118	0.79%	32.73%	G4SteppingManager::DefinePhysicalStepLength()
3232859	0.78%	33.51%	G4ParticleChange::UpdateStepForAlongStep()
3201266	0.77%	34.28%	G4eBremsstrahlungModel::SampleSecondaries()
3198988	0.77%	35.05%	G4VoxelNavigation::ComputeVoxelSafety()
3081196	0.74%	35.79%	CLHEP::RanluxEngine::flat()
2933359	0.71%	36.49%	G4MaterialPropertiesTable::GetProperty()
2918537	0.70%	37.20%	G4PolyconeSide::Intersect()
2881473	0.69%	37.89%	G4Tubs::Inside()
2879699	0.69%	38.58%	G4MaterialPropertyVector::GetProperty()
2708685	0.65%	39.23%	G4VoxelNavigation::VoxelLocate()
2708569	0.65%	39.88%	G4StepPoint::operator=()
2702742	0.65%	40.53%	G4Box::Inside()
2642777	0.64%	41.17%	G4PhysicsVector::GetValue()
2570738	0.62%	41.79%	G4ParticleChangeForTransport::UpdateStepForAlongStep()
2533828	0.61%	42.40%	G4Tubs::DistanceToIn()
2404980	0.58%	42.98%	G4MscModel::GeomPathLength()
2380731	0.57%	43.55%	G4MagErrorStepper::Stepper()
2375239	0.57%	44.12%	G4Track::GetVelocity()
2364408	0.57%	44.69%	G4VEmProcess::GetMeanFreePath()
2192185	0.53%	45.22%	G4IntersectingCone::LineHitsCone2()
2173750	0.52%	45.74%	G4MagInt_Driver::AccurateAdvance()
2138457	0.51%	46.25%	G4Box::DistanceToOut()
2101661	0.51%	46.76%	G4SandiaTable::GetSandiaCofPerAtom()
2073579	0.50%	47.26%	G4ParticleChange::Initialize()
2070889	0.50%	47.76%	G4ClassicalRK4::DumbStepper()
2023616	0.49%	48.24%	G4PropagatorInField::ComputeStep()
1982965	0.48%	48.72%	G4Mag_UsualEqRhs::EvaluateRhsGivenB()
1982311	0.48%	49.20%	G4PolyconeSide::Distance()
1925370	0.46%	49.66%	G4Box::DistanceToOut()
1921372	0.46%	50.12%	G4PolyconeSide::Inside()
1909913	0.46%	50.58%	std::_Rb_tree< >::lower_bound()
1843361	0.44%	51.02%	G4Cons::DistanceToIn()
1828376	0.44%	51.46%	G4Trd::Inside()
1804773	0.43%	51.90%	G4VDiscreteProcess::PostStepGetPhysicalInteractionLength()
1801818	0.43%	52.33%	_int_free
1752402	0.42%	52.75%	G4AffineTransform::G4AffineTransform()
1730562	0.42%	53.17%	G4VContinuousDiscreteProcess::PostStepGetPhysicalInteractionLength()
1693222	0.41%	53.58%	G4DisplacedSolid::Inside()
1670901	0.40%	53.98%	G4Sphere::DistanceToIn()
1648375	0.40%	54.37%	G4MscModel::SampleSecondaries()
1630064	0.39%	54.77%	G4VEnergyLossProcess::PostStepDoIt()

- Geant4.8.0.p01

- "*configuration which reproduces a typical LHC calorimeter*"

- atlasHEC.g4 :

  - 5000 events of 100 GeV pi-

  - ATLAS HEC calorimeter (Copper-LiquidArgon)
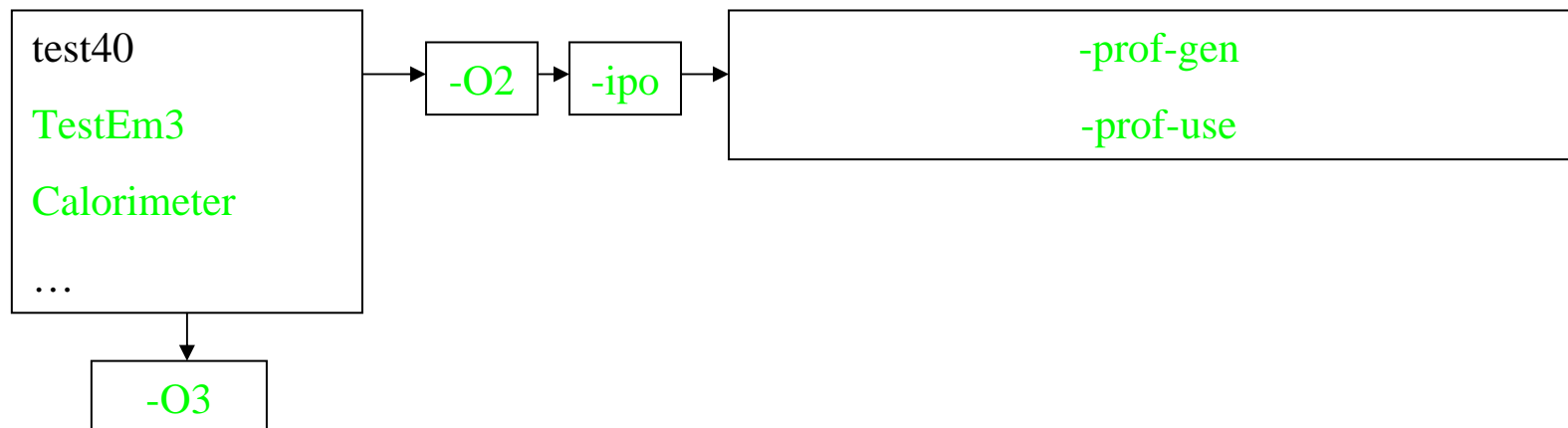
libraries[%]

geant4[%]

Function Summary

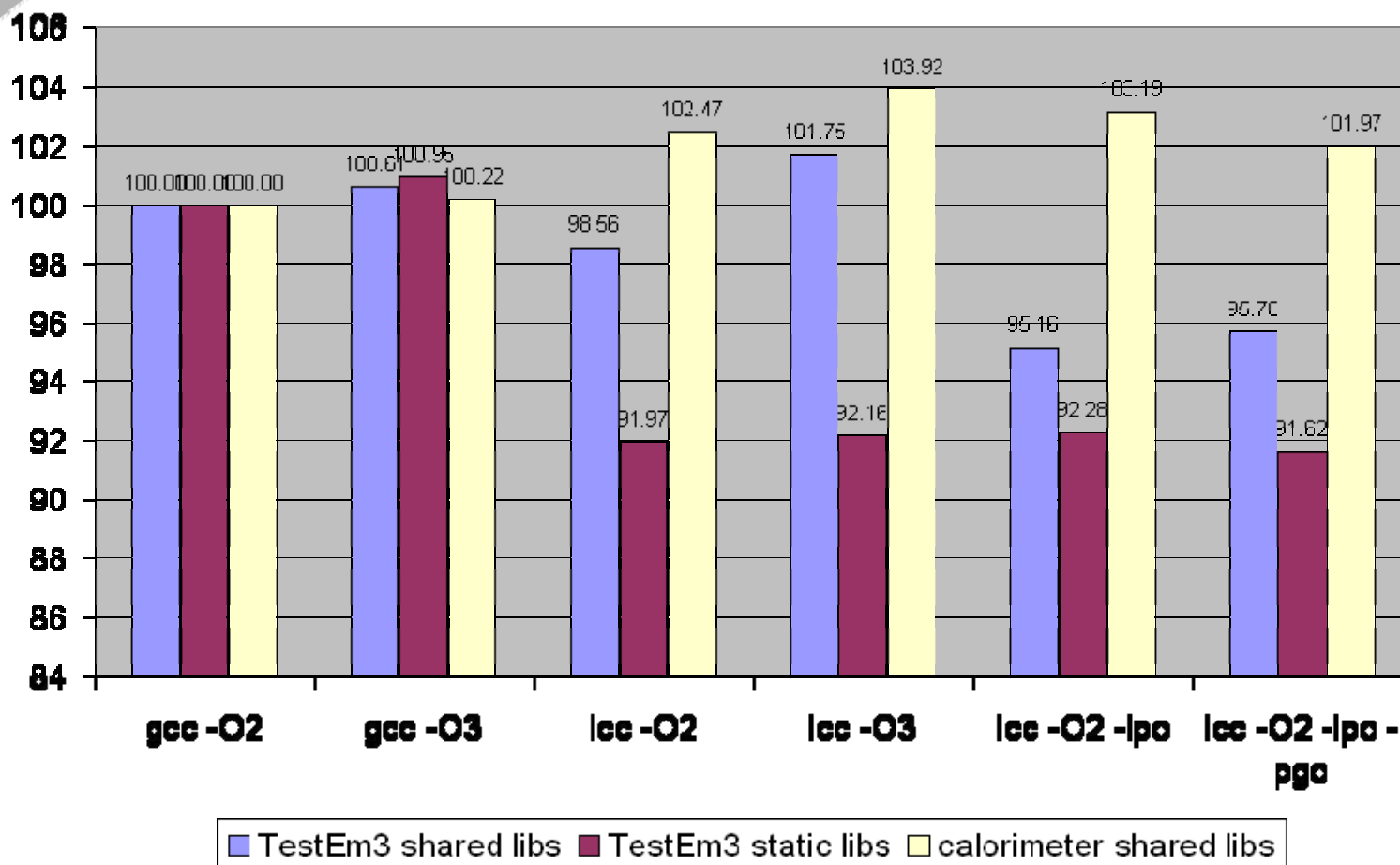| Samples	Self %	Total %	Function
43663318	6.07%	6.07%	??
14323092	1.99%	8.06%	G4eBremsstrahlungModel::SampleSecondaries()
13989279	1.94%	10.00%	G4UniversalFluctuation::SampleFluctuations()
10520122	1.46%	11.46%	G4MscModel::SampleCosineTheta()
10485807	1.46%	12.92%	G4Navigator::LocateGlobalPointAndSetup()
10151605	1.41%	14.33%	G4Transportation::AlongStepGetPhysicalInteractionLength()
9879567	1.37%	15.70%	G4Navigator::ComputeStep()
9477618	1.32%	17.02%	G4SteppingManager::SetInitialStep()
9415974	1.31%	18.33%	G4VEnergyLossProcess::AlongStepDoIt()
9217994	1.28%	19.61%	G4SteppingManager::Stepping()
8914560	1.24%	20.85%	G4KleinNishinaCompton::SampleSecondaries()
8807404	1.22%	22.07%	G4Navigator::LocateGlobalPointAndUpdateTouchableHandle()
7709725	1.07%	23.14%	G4SteppingManager::InvokePSDIP()
7634047	1.06%	24.20%	CLHEP::HepRotation::rotateAxes()
7459101	1.04%	25.24%	G4Quasmon::CalculateHadronizationProbabilities()
7408432	1.03%	26.27%	G4VEmProcess::PostStepDoIt()
7311983	1.02%	27.28%	__printf_fp
7178416	1.00%	28.28%	G4MscModel::SampleSecondaries()
7137088	0.99%	29.27%	G4QPDGCode::MakeQCode()
6739533	0.94%	30.21%	StatAccepTestSteppingAction::UserSteppingAction()
6693000	0.93%	31.14%	_int_malloc
6679076	0.93%	32.07%	StatAccepTestAnalysis::classifyParticle()
6494007	0.90%	32.97%	G4NavigationLevelRep::G4NavigationLevelRep()
6434676	0.89%	33.86%	G4SteppingManager::InvokeAlongStepDoItProcs()
6393189	0.89%	34.75%	G4HadronCrossSections::CalcScatteringCrossSections()
6052991	0.84%	35.59%	G4VEnergyLossProcess::PostStepDoIt()
5487814	0.76%	36.36%	G4SteppingManager::DefinePhysicalStepLength()
5473295	0.76%	37.12%	G4ElectroNuclearCrossSection::GetCrossSection()
5405793	0.75%	37.87%	G4MscModel::GeomPathLength()
5393849	0.75%	38.62%	G4Transportation::PostStepDoIt()
5114942	0.71%	39.33%	G4QPDGCode::GetNuclMass()
5044574	0.70%	40.03%	G4HadronicProcess::FillTotalResult()
5024798	0.70%	40.73%	StatAccepTestAnalysis::infoTrack()
4880028	0.68%	41.41%	G4ReplicaNavigation::BackLocate()
4662265	0.65%	42.05%	G4QPDGCode::GetQuarkContent()
4508388	0.63%	42.68%	G4QContent::GetSPDGCode()
4409611	0.61%	43.29%	G4VoxelNavigation::LevelLocate()
4403274	0.61%	43.90%	G4VMultipleScattering::GetContinuousStepLimit()
4088362	0.57%	44.47%	G4NormalNavigation::ComputeStep()
4081713	0.57%	45.04%	G4Transportation::AlongStepDoIt()
3890535	0.54%	45.58%	G4QHadron::DefineQC()
3837255	0.53%	46.11%	CLHEP::RanluxEngine::flat()
3809001	0.53%	46.64%	vfprintf
3775260	0.52%	47.17%	G4Navigator::ComputeSafety()
3681883	0.51%	47.68%	G4StepPoint::operator=()
3631515	0.50%	48.18%	G4SandiaTable::GetSandiaCofPerAtom()
3587519	0.50%	48.68%	G4PEEffectModel::SampleSecondaries()
3550782	0.49%	49.17%	G4TrackingManager::ProcessOneTrack()
3538891	0.49%	49.67%	G4MultipleScattering::TruePathLengthLimit()
3398061	0.47%	50.14%	G4HadronicProcess::GeneralPostStepDoIt()
3394506	0.47%	50.61%	G4VEmProcess::GetMeanFreePath()
3346945	0.47%	51.08%	G4QContent::operator-=()
3303436	0.46%	51.53%	G4Tubs::DistanceToOut()
3280931	0.46%	51.99%	G4BetheHeitlerModel::SampleSecondaries()
3275052	0.46%	52.45%	G4PhotoNuclearCrossSection::GetCrossSection()
3238652	0.45%	52.90%	G4Tubs::Inside()
3222026	0.45%	53.34%	G4ParticleChange::CheckIt()
3190136	0.44%	53.79%	G4QNucleus::G4QNucleus()
3181739	0.44%	54.23%	G4MscModel::SampleDisplacement()
2939523	0.41%	54.64%	G4LElastic::ApplyYourself()
2936645	0.41%	55.04%	G4ParticleChangeForTransport::UpdateStepForAlongStep()
2906598	0.40%	55.45%	G4PhysicsVector::GetValue()
2796143	0.39%	55.84%	G4IonTable::IsLightIon()

Further possible directions

- **iCC**

| test40 TestEm3 Calorimeter … | → | -O2 | → | -ipo | → | -prof-gen -prof-use |

(test40 → -O3)

- **GNU**

| test40 TestEm3 Calorimeter … | → | -O2 | → | -fprofile-generate -fprofile-use |

(test40 → -O3)
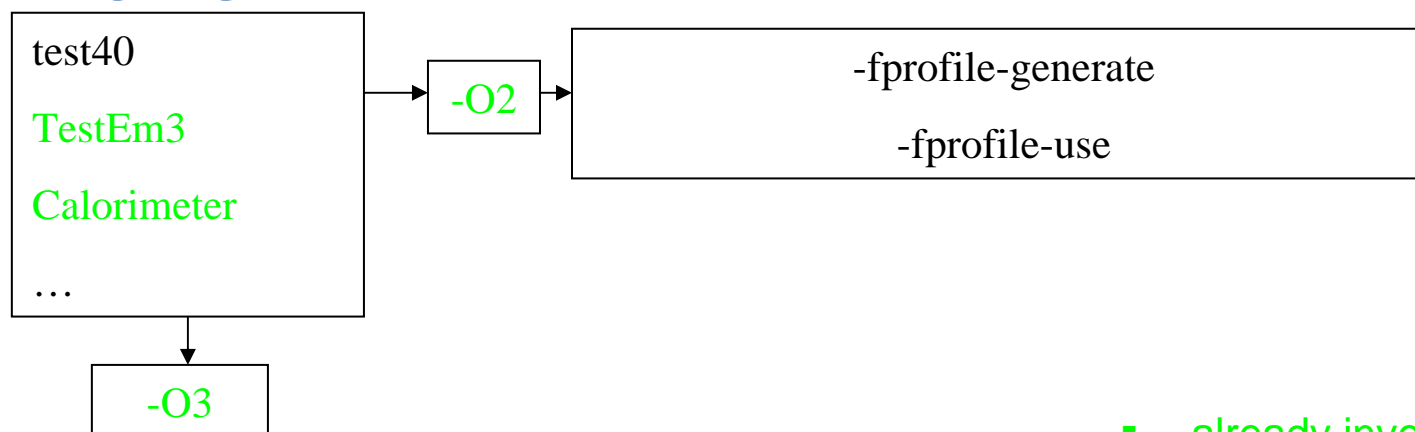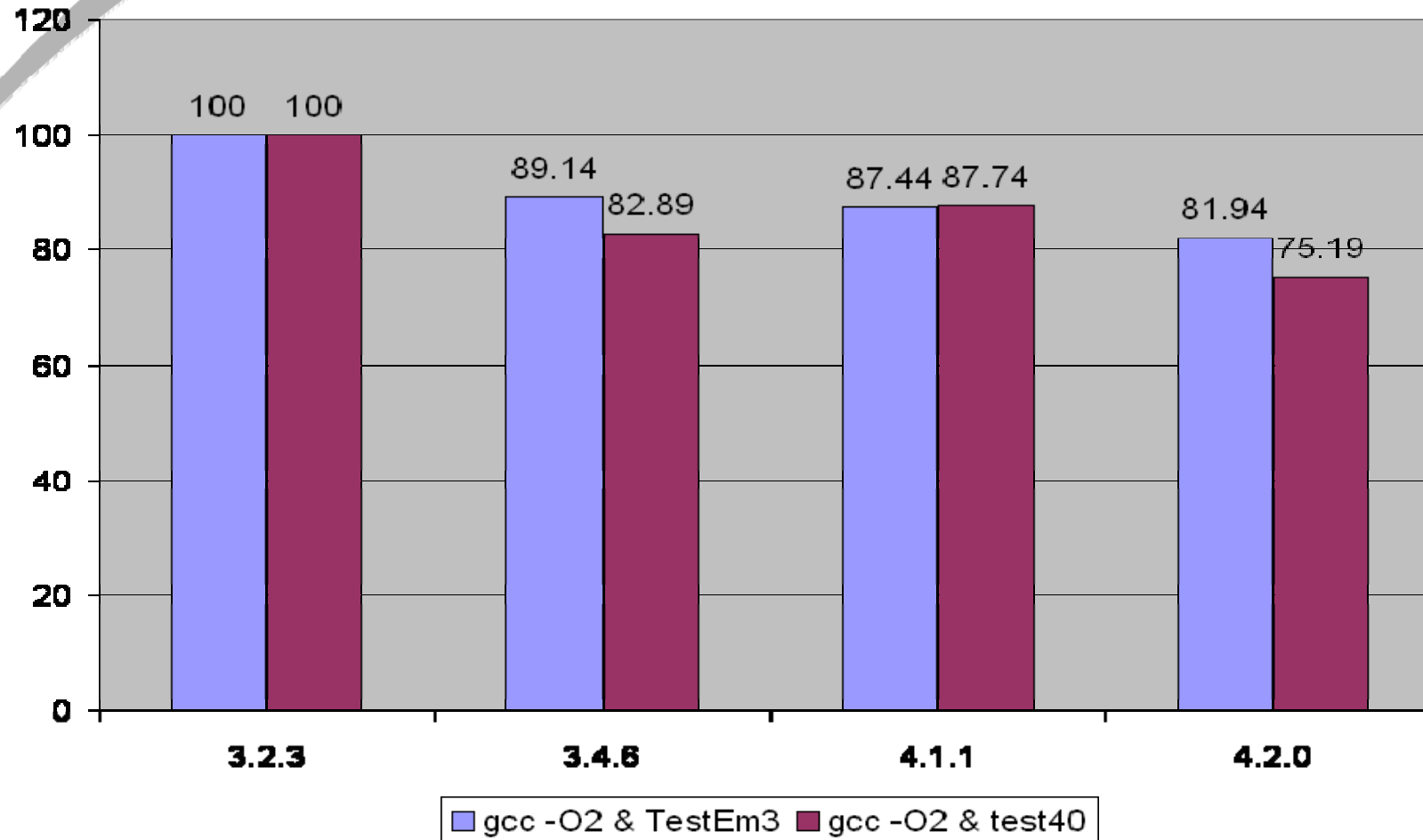
■ already investigated

TestEm3 & gcc-3.2.3 & icc 9.0

- scaled in time, smaller is better

gcc comparison

- scaled in time, smaller is better

G4 shared libs vs. static libs

TestEm3 real time[scaled]
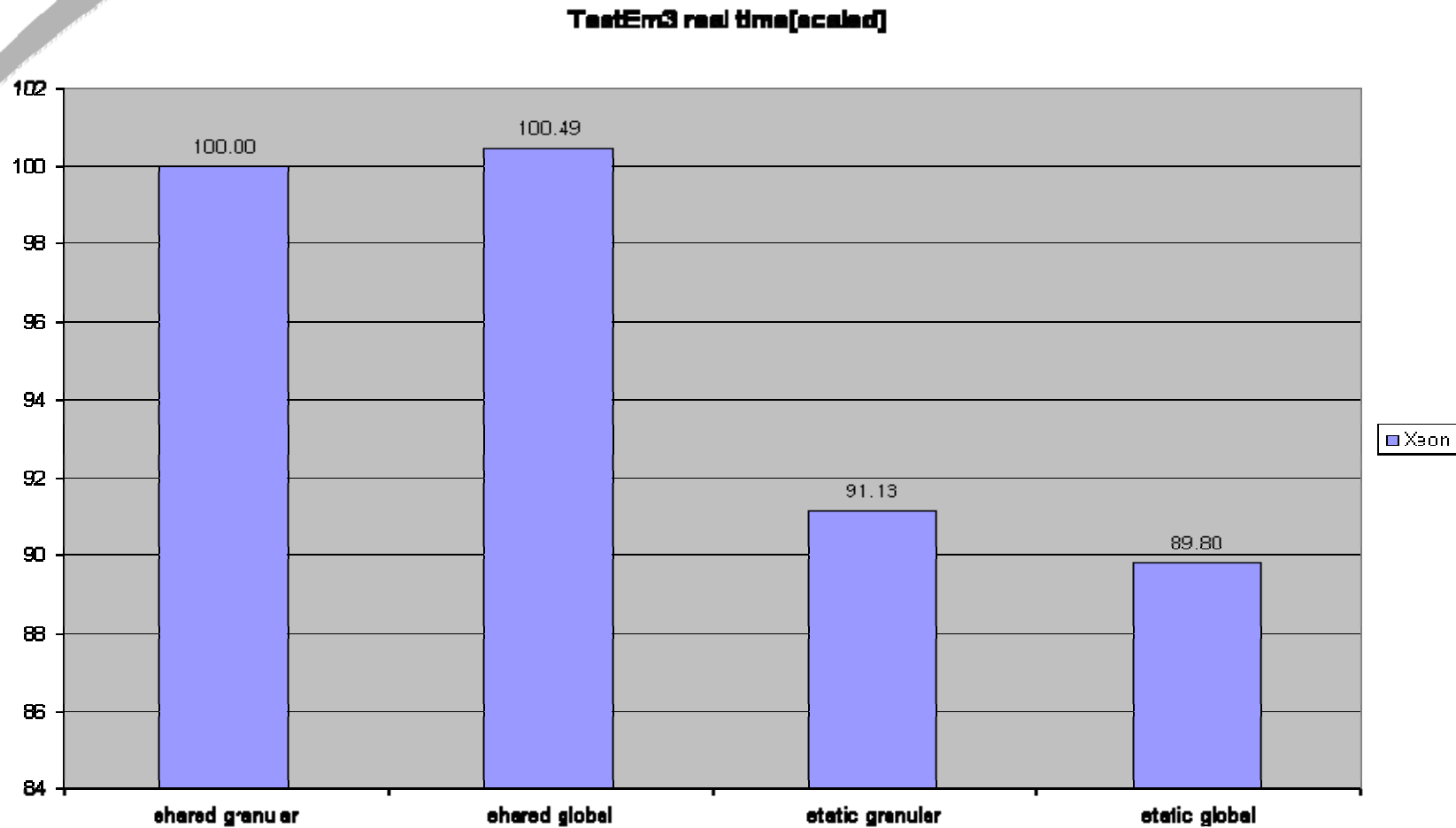
- scaled in time, smaller is better

- **Tool**
  - improve resolution of function names from shared libraries
  - number of function calls

- **Geant4 libs**
  - different compilers
    - gcc, icc, open64
  - different compiler options

- **32bit and 64bit mode**

Q&A?