Geant4 Version 10: Lessons learnt

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Forum on Concurrent Programming Models and Frameworks

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U.S. DEPARTMENT OF ENERGY
Office of Science

SLAC NATIONAL ACCELERATOR LABORATORY

Design Considerations: the process to G4 Version 10

- We first defined our **main design goals**:
  - Make efficient use of many-core technologies **reducing memory usage** w.r.t. MP, CoW, …
  - New Geant4 should be an **evolution** from current G4
  - User migration cost should be as **minimal** as possible
- A long (3 years) prototyping phase with well defined **incremental goals**:
  1. First define the technology
  2. Produce stand-alone code (e.g. branched from G4) showing main functionalities
  3. Demonstrate scalability of solutions
  4. Integrate in main code-base
  5. Release and patch

Design Considerations: the process to G4 Version 10

- MT code integrated into G4

- Public release
- All functionalities ported to MT

- Proof of principle
- Identify objects to be shared
- First testing

- API re-design
- Example migration
- Further testing
- First optimizations

- Further Refinements
- Focus on further performance improvements

Where to start from?

- In MC simulation events are independent, natural choice: event-level parallelism
  - **Requires all code to be thread-safe**, two options possible:
    1. Review each single class in G4
    2. Develop a general strategy that is valid everywhere
- Second option requires **long initial design/prototyping work** but it is more beneficial in the long run (thread-local-storage)
- After this general design phase we focused on reducing memory footprint (split-classes)

Thread-safety in Version 10.0

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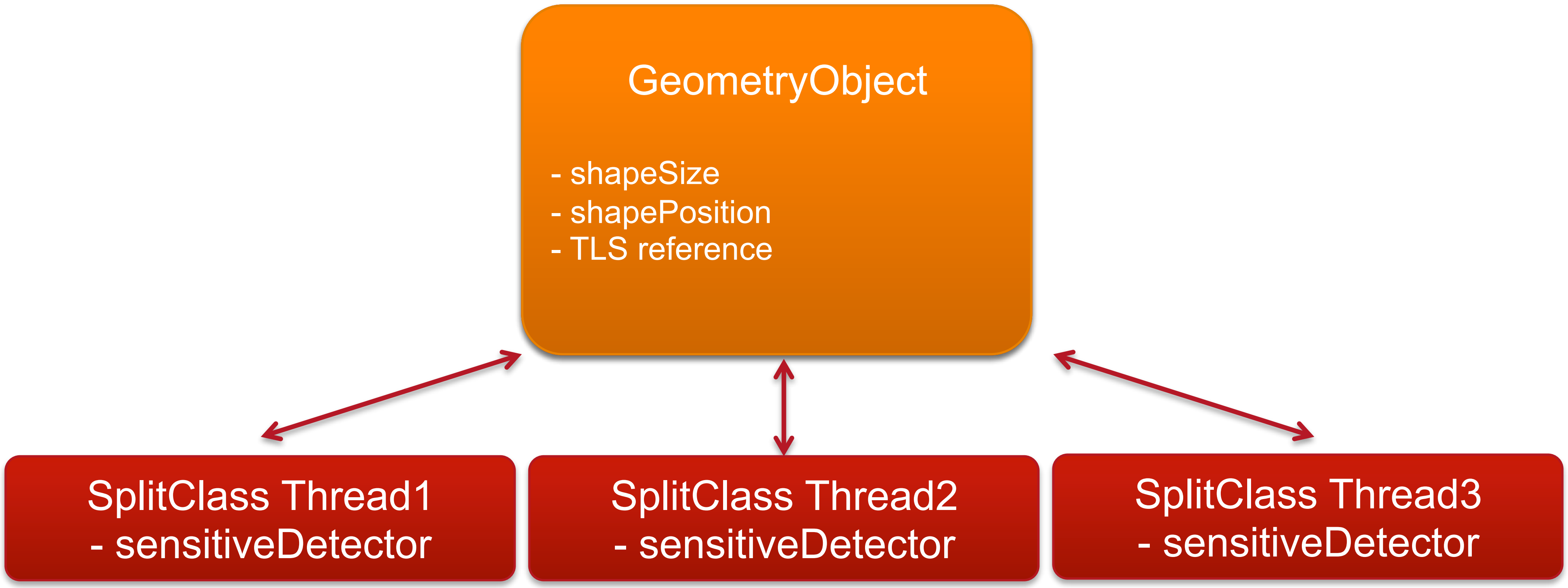
- Thread-safety implemented via **Thread Local Storage**
  - Managers (e.g. singleton) are basic components: "naturally" thread-local
- **"Split-class" mechanism:** reduce memory consumption
  - Read-only part of most memory consuming objects shared between thread: Geometry, Physics Tables
  - Rest is thread-private



Thread Local Storage

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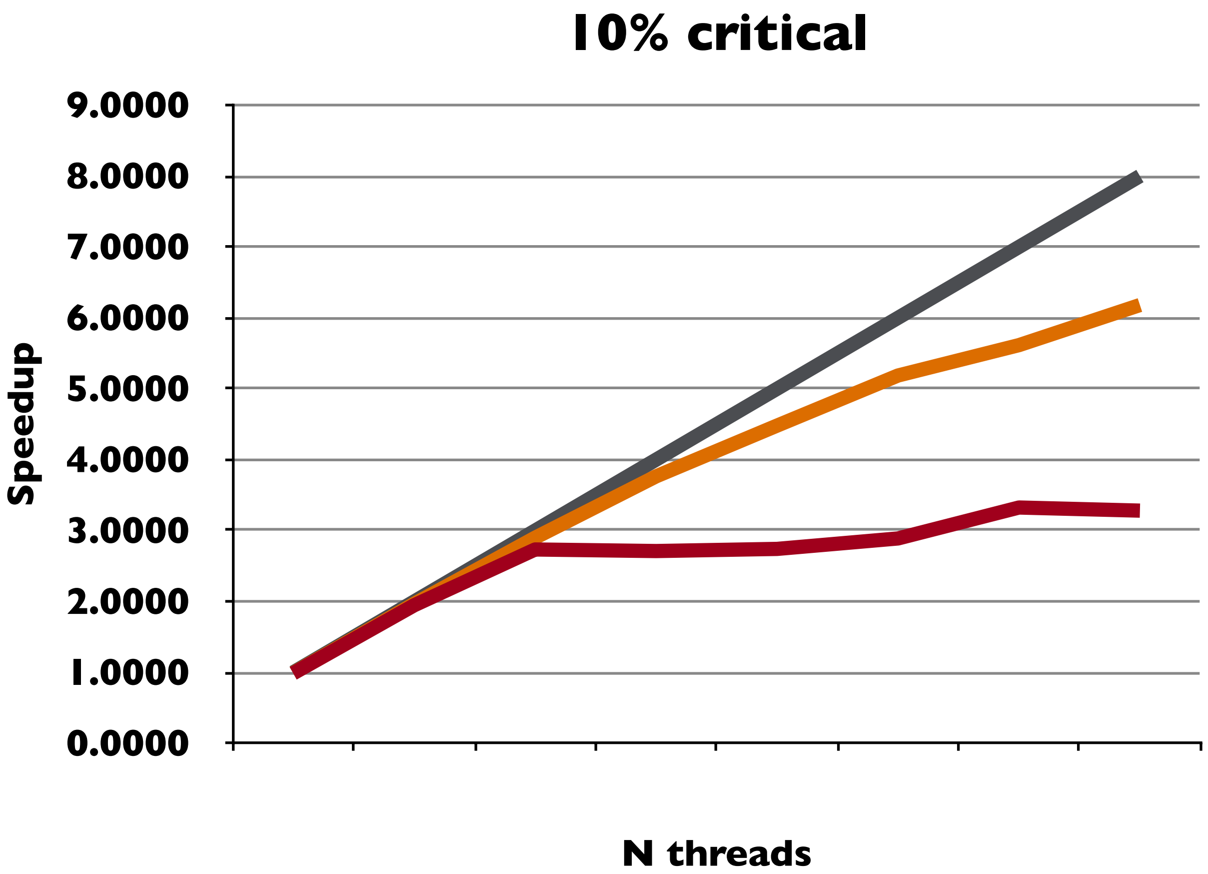
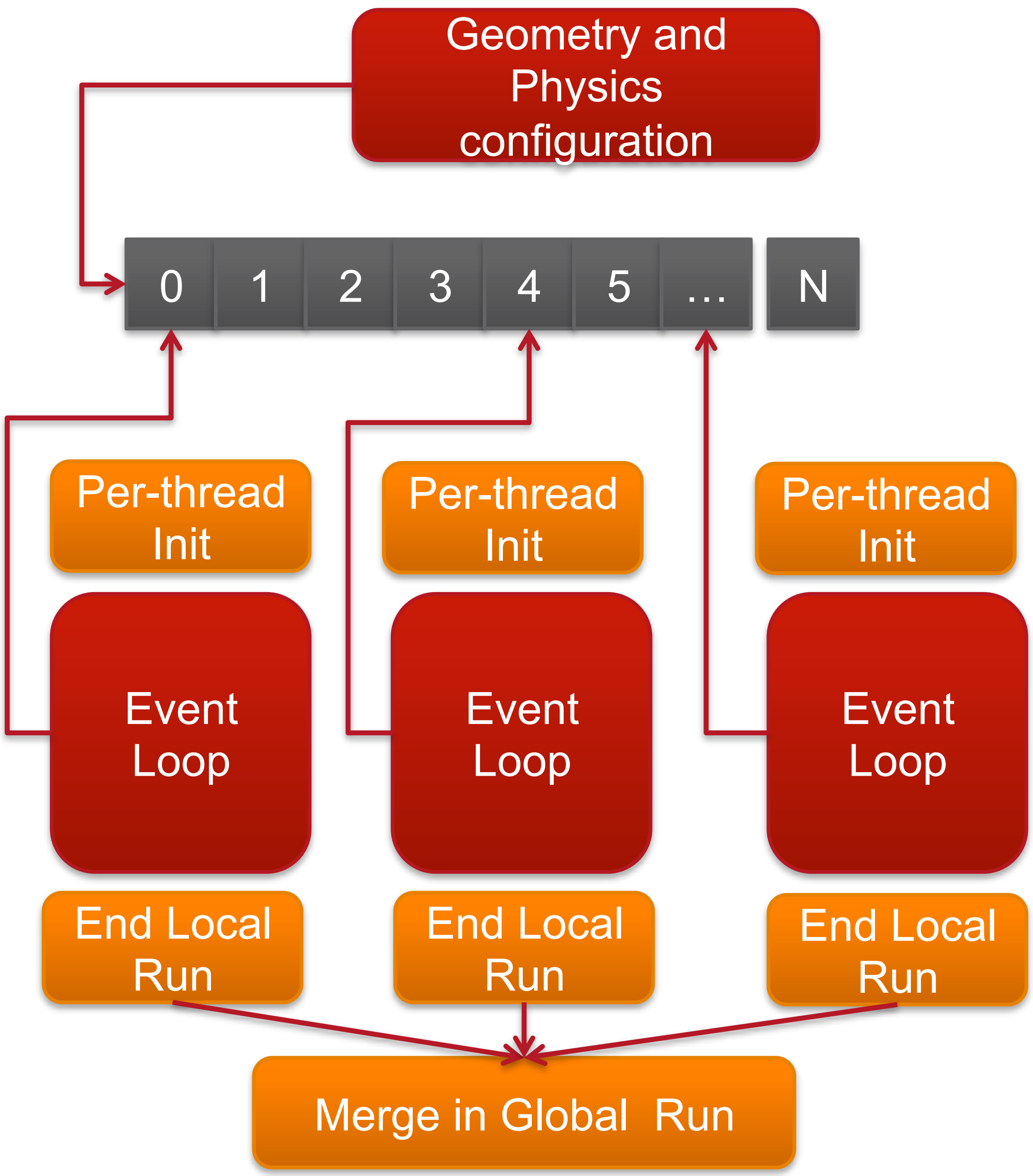


- Each (parallel) program has sequential components
  - **Protect access to concurrent resources**
- Simplest solution: use mutex/lock
- TLS: each thread has its own object (no need to lock)
  - **Supported by all modern compilers**
- Challenge: only simple data types for static/global variables can be made TLS
- Warning: hidden locks are important too (e.g. `operator new`, use of `std::strstream`)

NB: results obtained on toy application, not real G4

Multi-threading master/worker model



Per-event seeds pre-prepared in a "queue"

Threads compete for next event to be processes (new in ref-08)

Command line scoring and G4tools automatically merge results from threads

Did we get it right?

- Constantly review design and implementation choices with partners:
  - **Developer community:** dedicated mailing-list for discussions, twiki pages, in-depth face-to-face discussions
  - **User community**: release soon and often, setup a dedicated user-community forum (31 threads, 27 are related to prototypes)
  - **"Official" documentation**: conference proceeding, articles, manuals (extremely important also for developers)
- We are not expert in the sector: **collaboration with Computing Scientist**
  - Collaboration between physicists (authors of algorithms) and computing scientists (experts in how to efficiently implement them) is a key element of G4-MT success
  - It also helps in reducing typical physicists attitude to "reinvent the wheel"

Focus on important metrics

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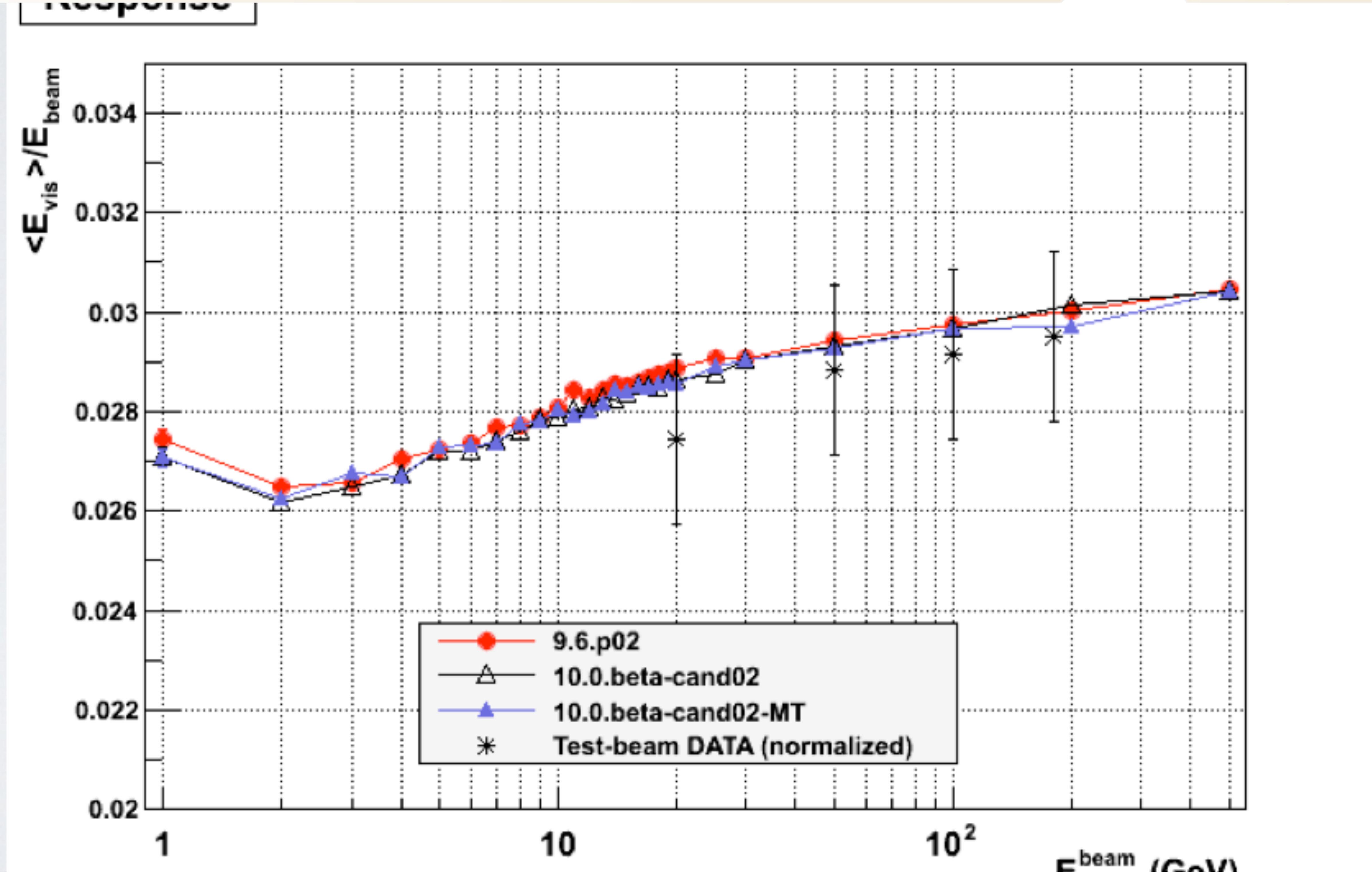
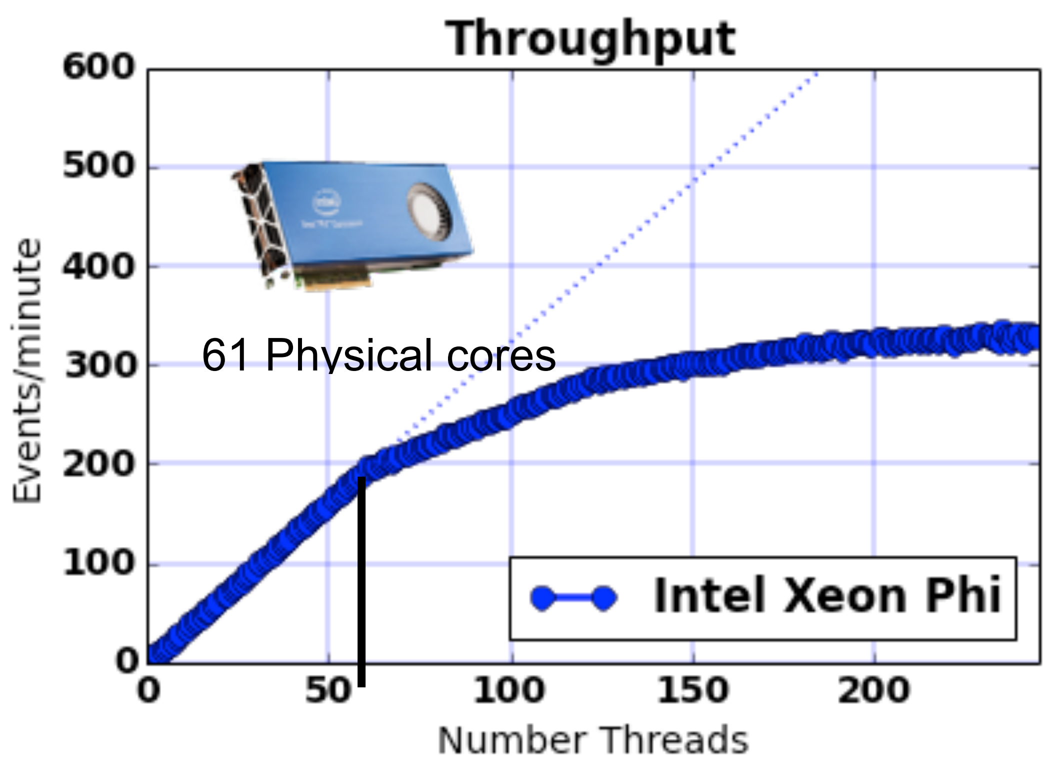
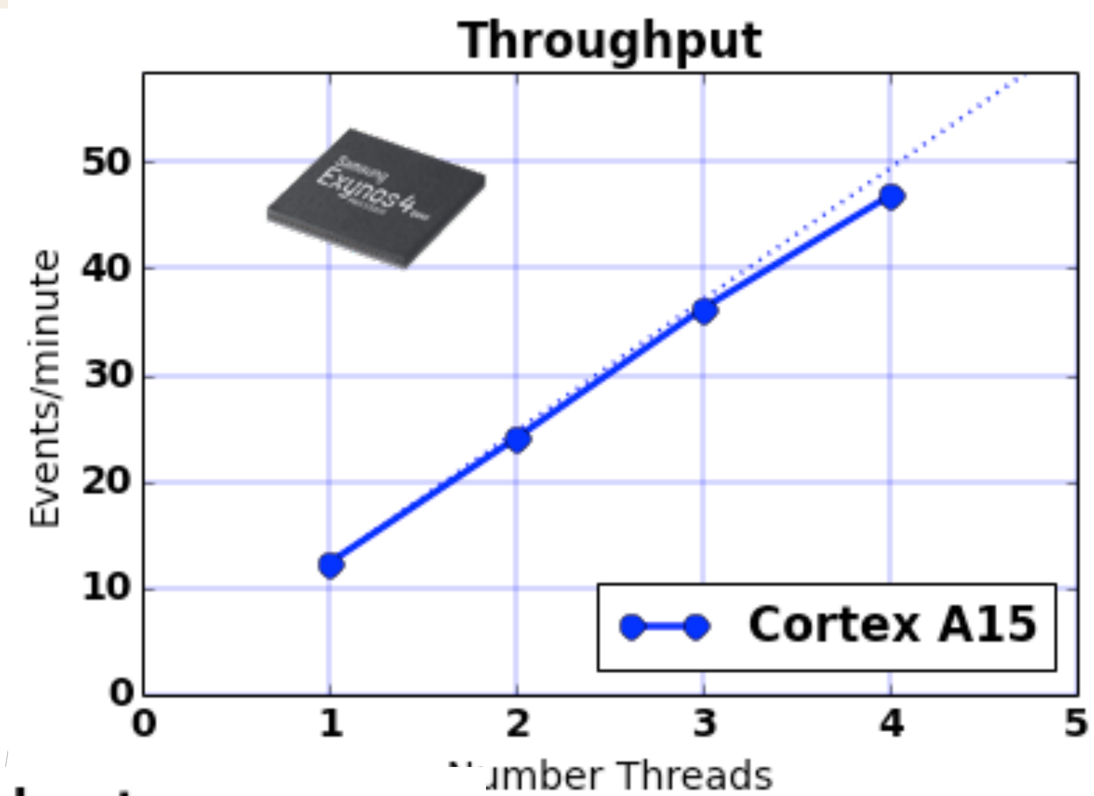
- Defined **very early** our goals and how to measure them:
  - Produce **physics results** equivalent to sequential code independently of number of threads and event simulation order: Strong Reproducibility (much more difficult than what it sounds)
  - Two main metrics: **linearity of speedup**; **memory reduction**
  - Define immediately few test-benches (SimplifiedCalorimeter and FullCMS), independent group responsible for monitoring
- We have learned a lot from **using very early different hw and sw systems**: x86_64, MIC, ARM, Atom architectures
  - Linux, Mac OS X
  - Initial plan included also WIN, on-halt due to man power, challenging due to non POSIX standards
- **Measure often:** at least once per month

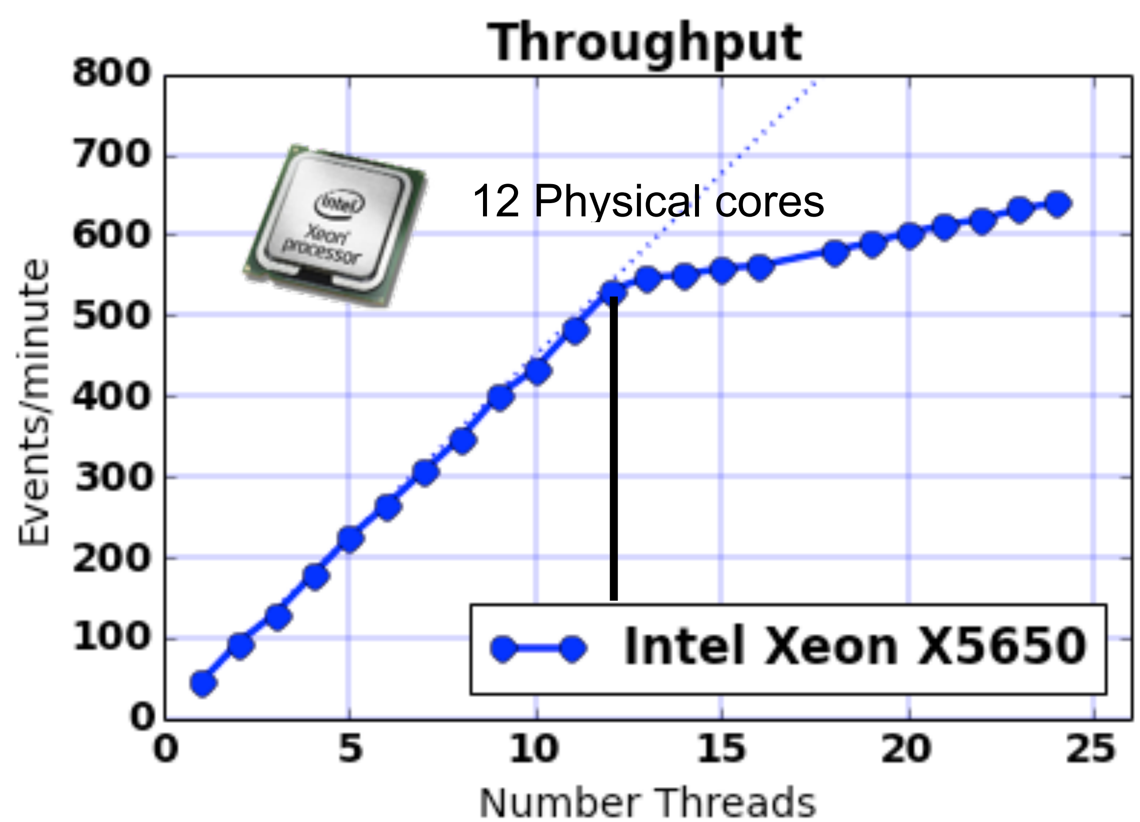
MT libs Vs SEQ libs



Performances





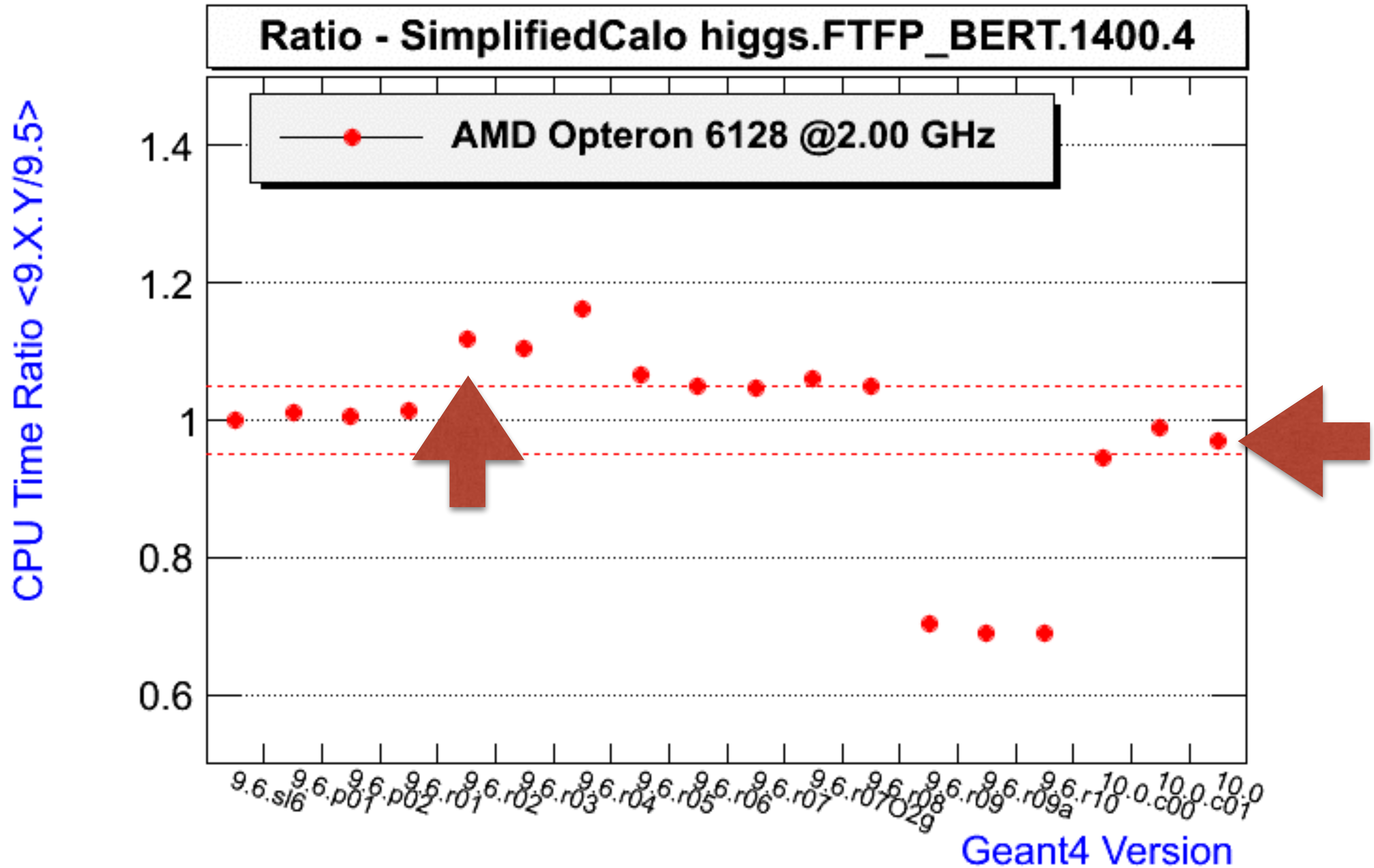


Absolute performances

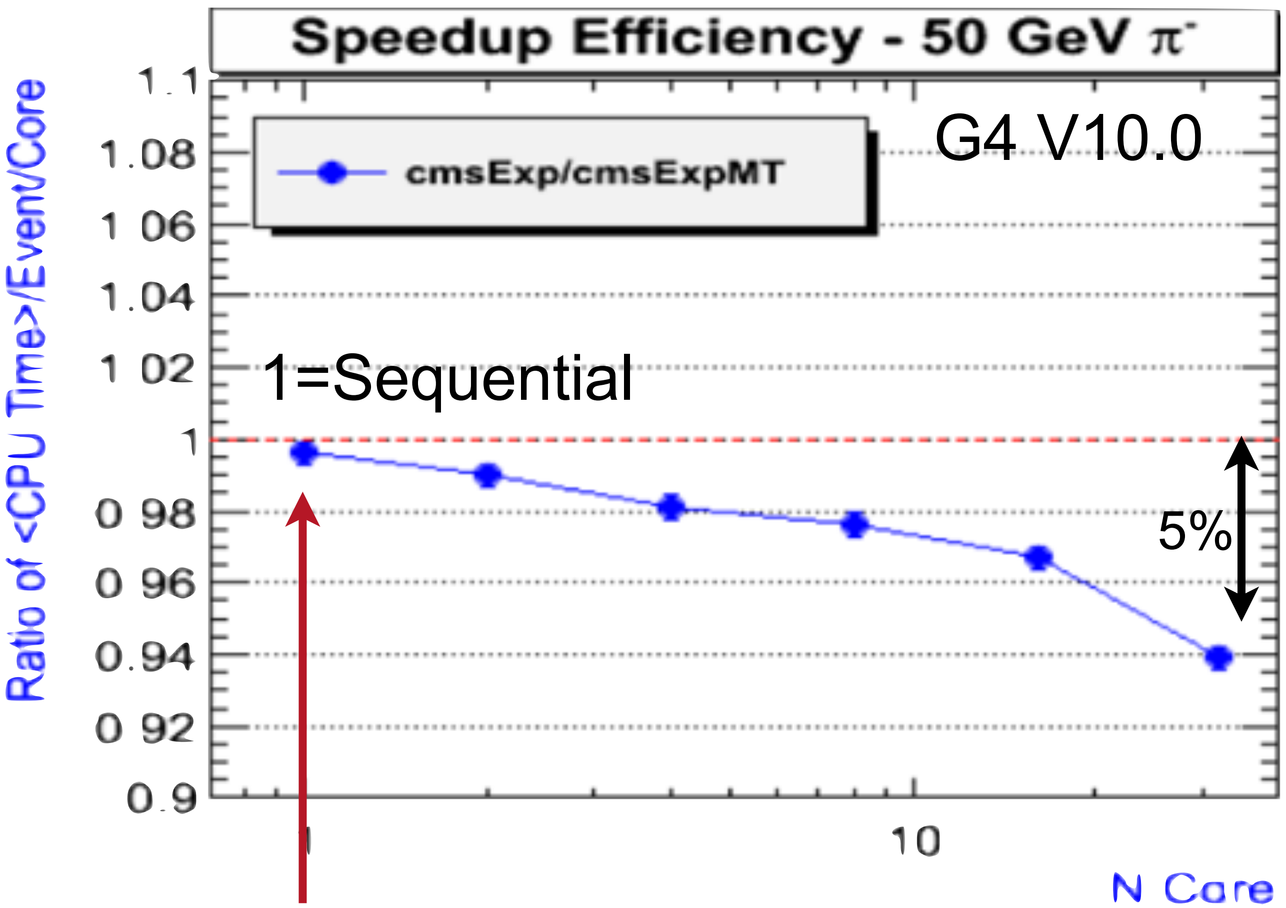
- We did expect a penalty for MT (e.g. performances 1-thread < sequential): due to TLS "machinery"
  - Challenge: **understand TLS details**, relatively new feature and documentation not always complete/clear.
- All initial performance issues **have been solved:**
  - There is only very little CPU penalty for MT builds
  - TLS is very powerful when used correctly, but should not be over-used

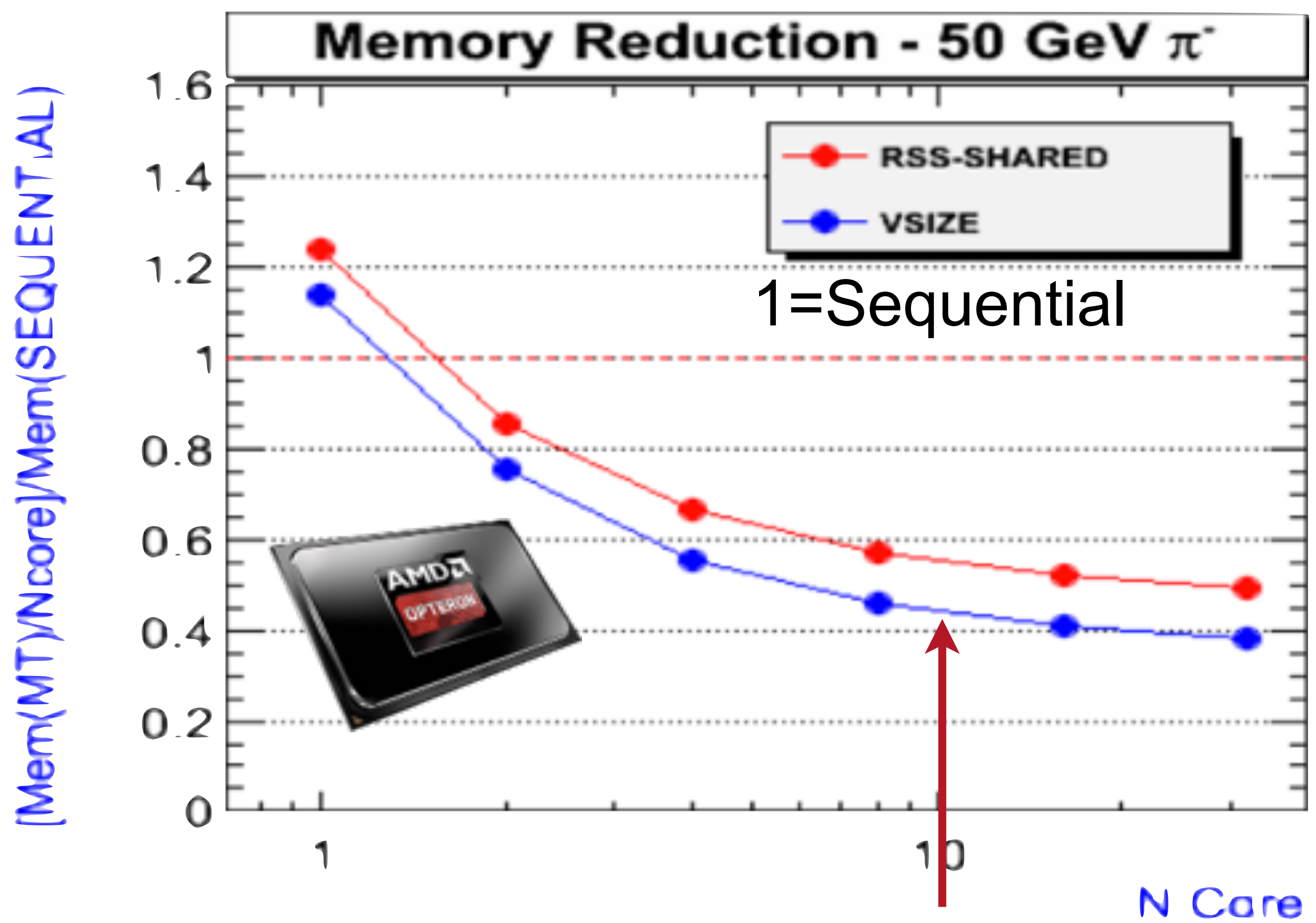
- Improvements in MT often brought benefits **also to sequential applications** (V10.0 w/ improved physics, MT functionalities, is faster than previous releases):
  - Re-arranging memory layout of geometry and physics (split-classes) bring some benefits in some cases (improve cache hit ratio)
  - Forced us to review several areas of our code
  - Would have more difficult with a separate "code-base" or using ad-hoc technologies/ languages

Benefits of MT developments for sequential code



Comparing with sequential





1 thread =>
Overhead for MT
Very small CPU penalty
~1%

10 threads =>
50% memory w.r.t.
10 sequential instances

Tools

- Finding right tools to develop MT code is a **challenge:**
  - **Development**: IDE with integrated GDB sessions are useful (but not full support for TLS), use coverity to fix possible defects, extensive use of CDash/CTest
  - **Debug**: we could not find any tool specifically designed to help debug MT applications
    - Most challenging aspect: crashes are non-reproducible, stack-traces are not always useful
    - Need a lot of experience: often developers ask the "experts" to re-run and debug
    - DRD is very useful for data-race identification (some experience needed to interpret output)
  - **Performances/profiling:** simple benchmarking is very useful if done often, full profiling tools need to be MT aware (OpenSpeedShop, Gooda)
  - Interesting lesson: typical "sequential" tricks to speed up simulations (e.g. caching calculations), may be not be so beneficial with many threads (increase hw cache misses). How to define tradeoff?
- G4 comes with extensive set of tests/examples (240 are run nightly in cdash), earlier MT migration would have helped to spot issues/bug earlier (lesson learnt: some sort of **test-driven development** would have been beneficial)

Gooda Example

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Reports

- reports/Sample
- reports/G4MT-new
- reports/G4MT-old

reports/G4MT-new Hotspots

Cycles Samples

Enter search term

process path	module path	unhalted_core_cycles		uops_retired:stall_cycles		instruction_retired	uops_retired:any
		8245843	(100%)	5703358	(69%)	3905966	4766639
ParFullCMS		8229714	(99%)	5654865	(68%)	3900553	4757241
aggregated_kernel_object		91525	(1%)	111330	(121%)	17110	28074
vmlinux		4869	(0%)	40659	(835%)	1492	4067
puppet		1431	(0%)	855	(59%)	556	723
perf		1401	(0%)	979	(69%)	563	881
sshd		934	(0%)	460	(49%)	873	1107
kworker/9:0		358	(0%)	248	(69%)	87	90
khugepaged		308	(0%)	190	(61%)	71	113
kworker/7:0		308	(0%)	234	(75%)	56	90
kworker/0:0		298	(0%)	190	(63%)	48	83
kworker/14:2		278	(0%)	285	(102%)	56	105
kthreadd		268	(0%)	234	(87%)	40	113

Cycles Samples

Enter search term

function name	unhalted_core_cycles		uops_retired:stall_cycles		instruction_retired	uops_retired:any	load_latency	
	8245843	(100%)	5703358	(69%)	3905966	4766639	2745332	(33%)
G4PhysicsVector::Value(do…	249801	(3%)	183440	(73%)	81361	96333	157004	(62%)
G4ElasticHadrNucleusHE::H…	175220	(2%)	110935	(63%)	119668	177152	2405	(1%)
G4Navigator::LocateGlobal…	190355	(2%)	141634	(74%)	59378	74117	144841	(76%)
G4PolyconeSide::DistanceA…	134038	(1%)	80485	(60%)	99852	125190	14410	(10%)
G4SteppingManager::Define…	131792	(1%)	89575	(67%)	79845	87085	75913	(57%)
G4CrossSectionDataStore::…	121696	(1%)	78271	(64%)	73528	96325	73975	(60%)
CLHEP::MTwistEngine::flat…	107107	(1%)	60097	(56%)	89551	93810	30359	(28%)
G4ClassicalRK4::DumbStepp…	82552	(1%)	37933	(45%)	113510	131667	2723	(3%)
G4Navigator::ComputeStep(…	110755	(1%)	76064	(68%)	52331	68123	28749	(25%)
G4VoxelNavigation::Comput…	113825	(1%)	80083	(70%)	50370	58626	62875	(55%)

function name	instruction_starvation		bandwidth_saturated		branch_misprediction		store_resources_saturated		instruction_latency		exception_handling	
	4665713	(56%)	80157	(0%)	522052	(6%)	204496	(2%)	1724700	(20%)	41728	(0%)
G4PhysicsVector::Value(do…	102099	(40%)	3478	(1%)	16477	(6%)			72405	(28%)	606	(0%)
G4ElasticHadrNucleusHE::H…	3021	(1%)	70	(0%)	884	(0%)	467	(0%)	123127	(70%)	1660	(0%)
G4Navigator::LocateGlobal…	101920	(53%)	1958	(1%)	9192	(4%)	7890	(4%)	25192	(13%)	586	(0%)
G4PolyconeSide::DistanceA…	10643	(7%)	1153	(0%)	6291	(4%)	20	(0%)	58860	(43%)	636	(0%)
G4SteppingManager::Define…	68719	(52%)	358	(0%)	7225	(5%)	3597	(2%)	15542	(11%)	407	(0%)
G4CrossSectionDataStore::…	36391	(29%)	258	(0%)	4541	(3%)	21048	(17%)	13356	(10%)	318	(0%)
CLHEP::MTwistEngine::flat…	41231	(38%)	179	(0%)	7622	(7%)			15185	(14%)	447	(0%)
G4ClassicalRK4::DumbStepp…	9948	(12%)	30	(0%)	2335	(2%)	6141	(7%)	17739	(21%)	199	(0%)
G4Navigator::ComputeStep(…	103898	(93%)	626	(0%)	9063	(8%)	298	(0%)	11041	(9%)	417	(0%)
G4VoxelNavigation::Comput…	55998	(49%)	745	(0%)	8238	(7%)	4074	(3%)	11538	(10%)	398	(0%)

Technology Choices

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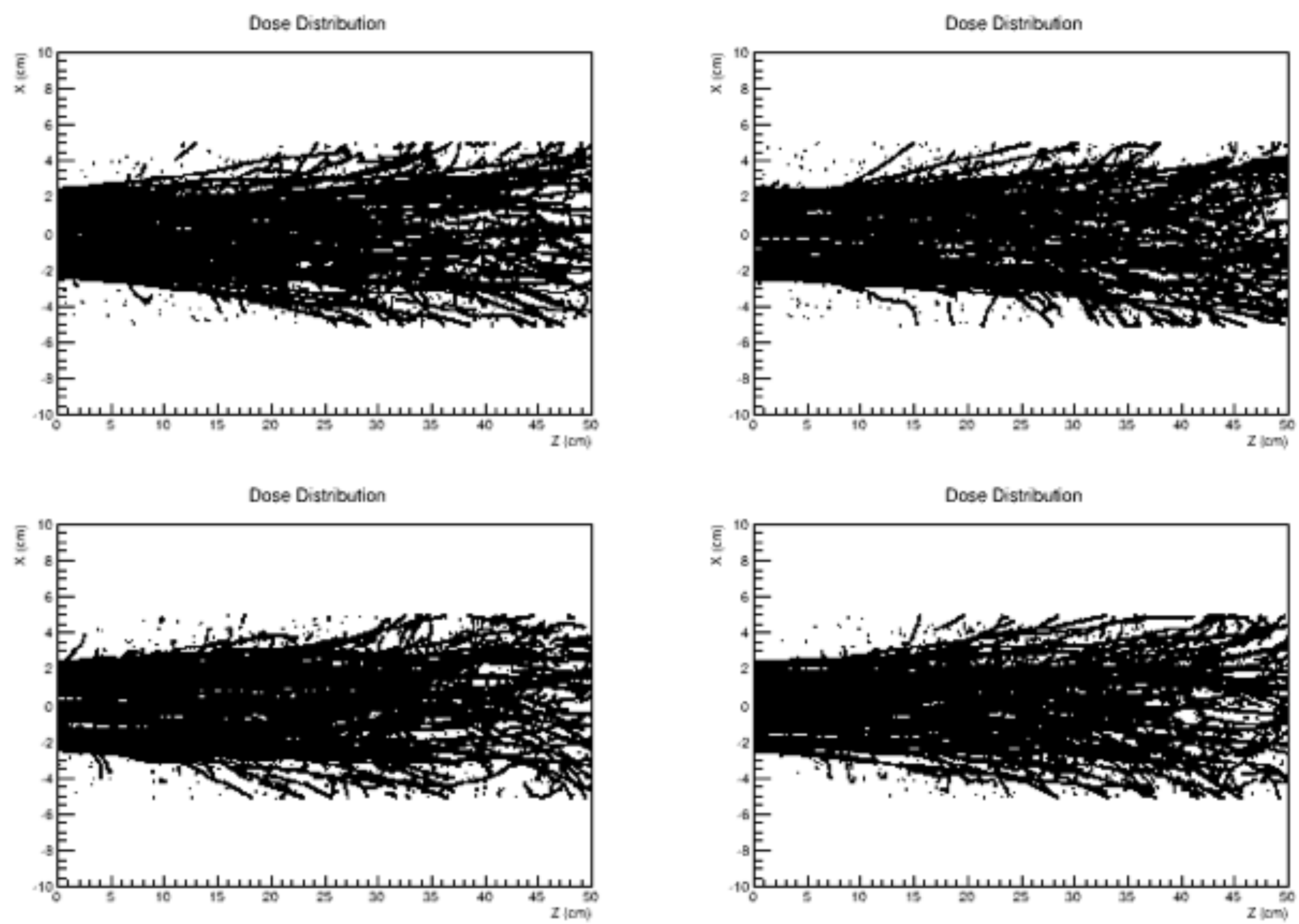
- We did **quite conservative** (sw) technology choices:
  - Use only POSIX standard (e.g. pthreads)
  - Use only compiler supported features (e.g. TLS)
- We believe these are **good choices:**
  - Almost trivial to port to new architecture (e.g. MIC porting done in few days)
  - Allow for **integration with "frameworks"** (provided that are compatible w/ standards): we have examples integrating MPI and TBB
  - Remember Geant4 is a toolkit integrated in larger (experimental) frameworks, not the other way around
- Very important: since these are standards, lots of example and documentation, lots of experience from other fields

Heterogeneous parallelism: MPI based G4MT

- **MPI based parallelism** available in Geant4
  - MPI works together with MT

Example:
4 MPI jobs
2 threads/job
MPI job owns histogram

Next Step:
Host + MIC simulation
Based on MPI



What's next?

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- **Further reduce memory consumption.** Thumb-rule: fit complex simulations on accelerators w/ O(100) threads and O(GB) memory
  - Warning: minimize memory usage can sometime **conflict** with other performance considerations (e.g. reduce memory "churn" may not always be thread-safety)
  - In our experience **profiling guided optimizations** are very effective: run profiling tools, identify top offender, work on them, repeat
- Further CPU benefits will come looking at single algorithms for new parallelization opportunities

Kind of Conclusions: My vision for Geant4 Version 11.0 :-)