GeantV

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HEP Software Foundation Workshop

LAL, May 2 – 4, 2016

Outline

- **GeantV**ectorized
  - Challenges, ideas, goals
- Main components
  - Geometry, physics, propagation in field, scheduler
- Development- different components in different stages
- Performance and benchmarks
  - Vectorization: overheads vs. gains
  - Geometry and physics performance: CPU and acceleratorsbenchmarks
- Results on parts, simple setups and full detector

The challenge

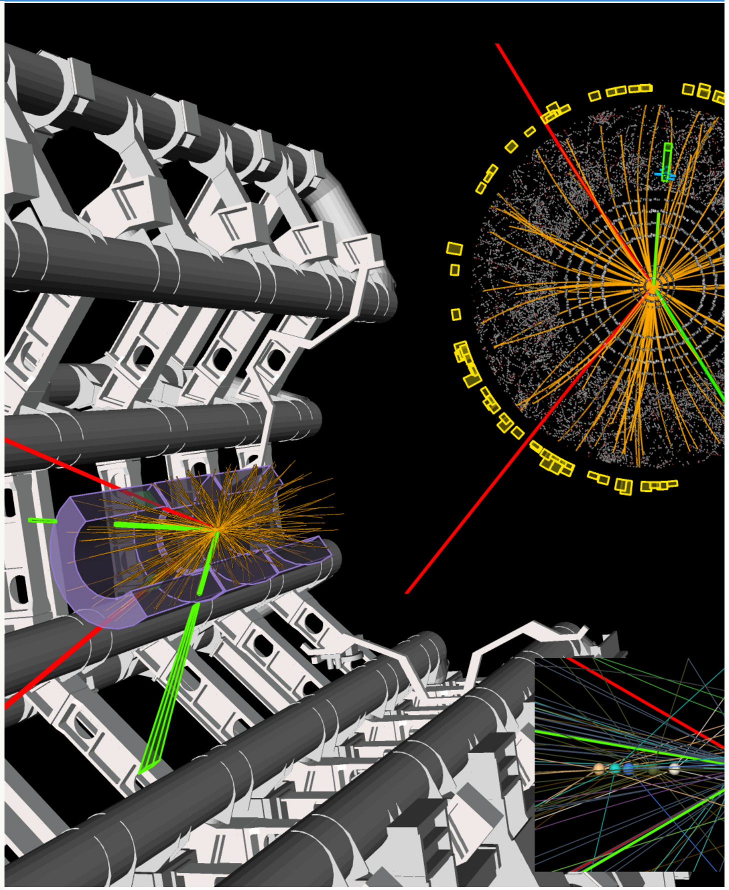
Goal of improving performance by a factor between 2.5 and 5 for large HEP detectors

Parts of transport of particles

- Navigating in complex geometries - millions of volumes
- Interactions using physics models,
- Propagation in EM field

Strongly CPU-bound, but must also generate user-determined output (hits & 'truth' information)

The LHC uses about 50% of its distributed GRID power for detector simulation



http://atlas.ch

The ideas

- Transport particles in groups (vectors) rather than one by one
  - Group particles by geometry volume or same physics
  - No free lunch: data gathering overheads < vector gains
- Dispatch SoA to functions with vector signatures
  - Use backends to abstract interface: vector, scalar
  - Use backends to insulate technology/library: Vc, Cilk+, VecMic, …
- Redesign the library and workflow to target fine grain parallelism
  - CPU, GPU, Phi, Atom, …
  - Aim for a 2.5x-5x faster code, understand hard limits for more

```
distance( double &);
```

Scalar interface

```
distance( vector_type  &);
```

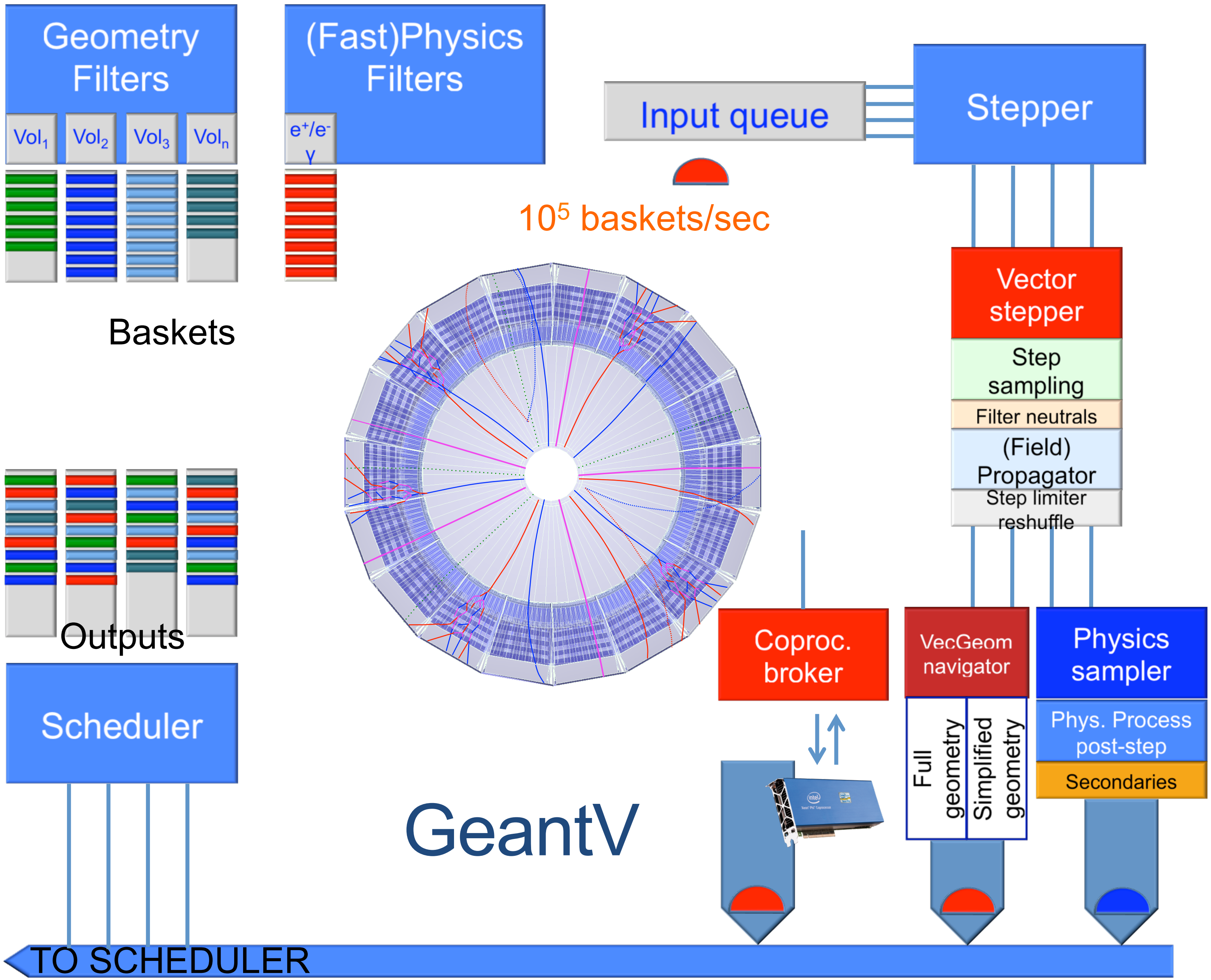
Vector interface

```
template<class Backend>
Backend::double_t
common_distance_function( Backend::double_t input )
{
   // Single kernel algorithm using Backend types
}
```

```
struct ScalarBackend
{
   typedef double double_t;
   typedef bool   bool_t;
   static const bool IsScalar=true;
   static const bool IsSIMD=false;
};
// Functions operating with backend types
```

```
struct VectorVcBackend
{
   typedef Vc::double_v double_t;
   typedef Vc::double_m bool_t;
   static const boolIsScalar=false;
   static const bool IsSIMD=true;
};
// Functions operating with backend types
```

code.compeng.uni-frankfurt.de/projects/vc


Geometry Filters
Vol_1 Vol_2 Vol_3 Vol_n
(Fast)Physics Filters
e^+/e^- γ
Baskets
Input queue
Stepper
10^5 baskets/sec
Vector stepper
Step sampling
Filter neutrals
(Field) Propagator
Step limiter reshuffle
Outputs
Scheduler
GeantV
Coproc. broker
VecGeom navigator
Full geometry
Simplified geometry
Physics sampler
Phys. Process post-step
Secondaries
TO SCHEDULER

Performance & Benchmarks

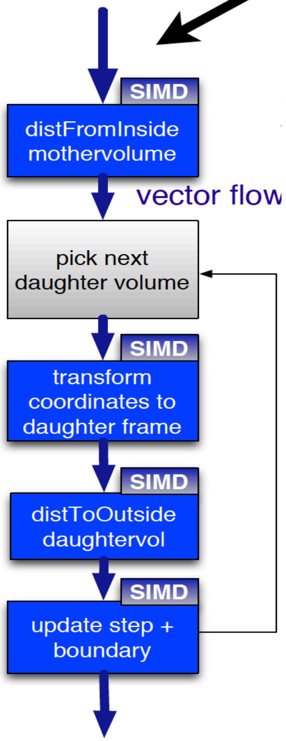
- Computing performance is a raison d’etre for GeantV
- Almost every component/class has a test and a benchmark for scalar and vector performance
  - Automated test, which must be run for each solid
  - Individual physics model sampling methods
- Benchmarks for
  - Navigation in simple and full detector geometries
  - ‘Full’ simulation using all integrated components

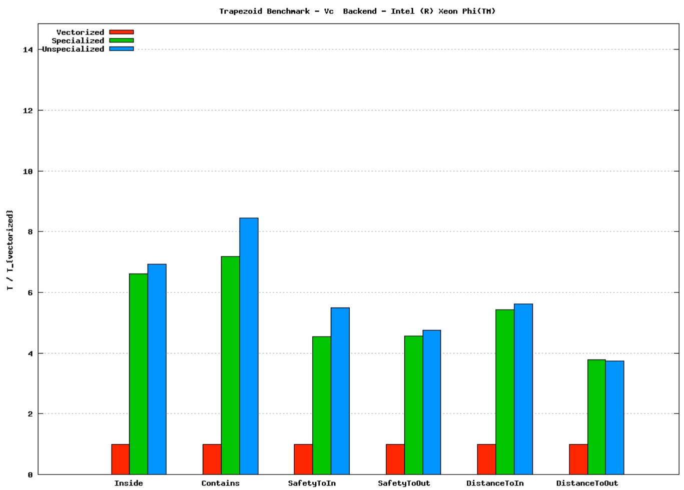
Geometry solid performance

- Geometry is 30-40% of the total CPU time in Geant4
- Vectorized geometry algorithms to take maximum advantage of SIMD
- Benchmark each method against implementations in Root, Geant4 and USolids library
- Performance gains also in scalar mode for some cases
- Testing the same on GPU

Speedup vs Number of particles	16 particles	1024 particles	SIMD max
Intel Ivy-Bridge (AVX)	2.8	4	4
Intel Haswell (AVX2)	3	5	4
Intel Xeon Phi (AVX-512)	4.1	4.8	8

Overall performance for a simplified detector vs. scalar ROOT/5.34.17

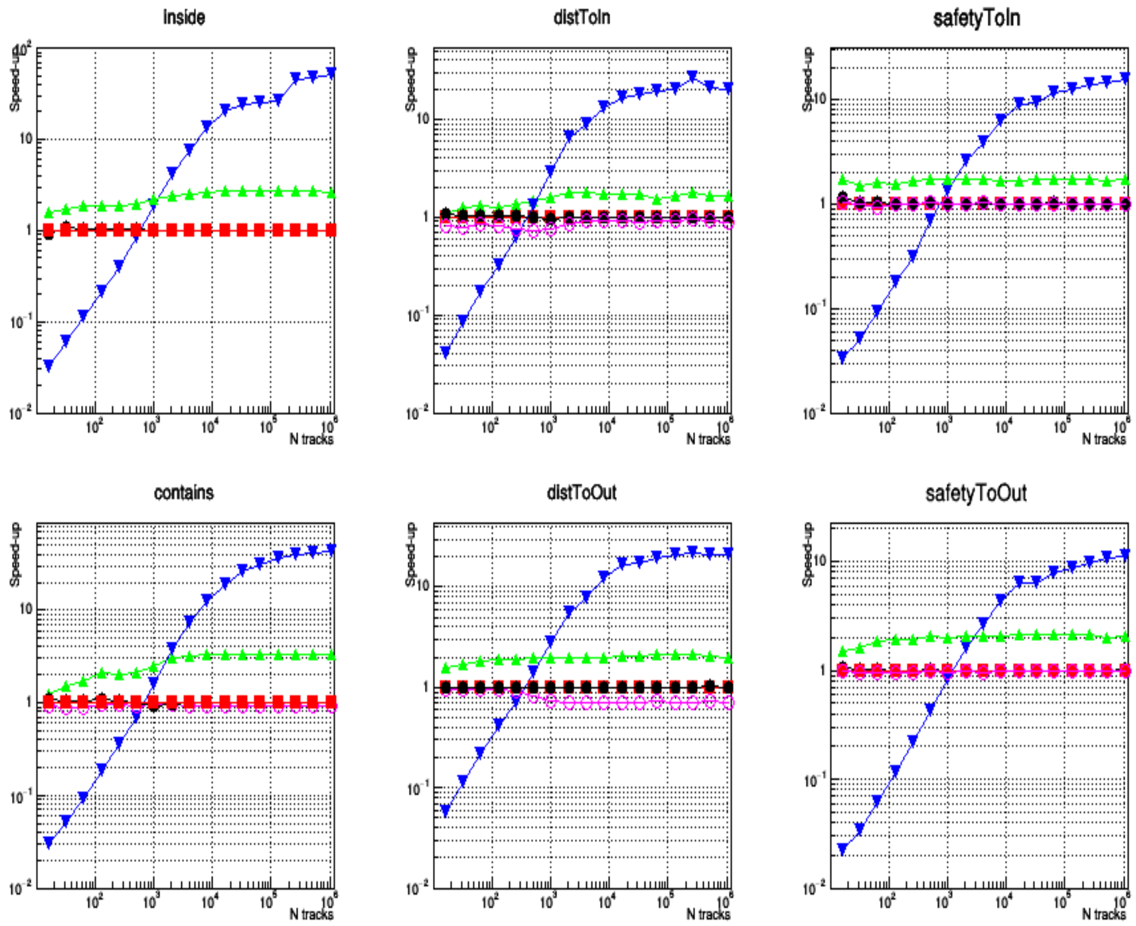




Vectorization performance for trapezoid shape navigation (Xeon®Phi® C0PRQ-7120 P)

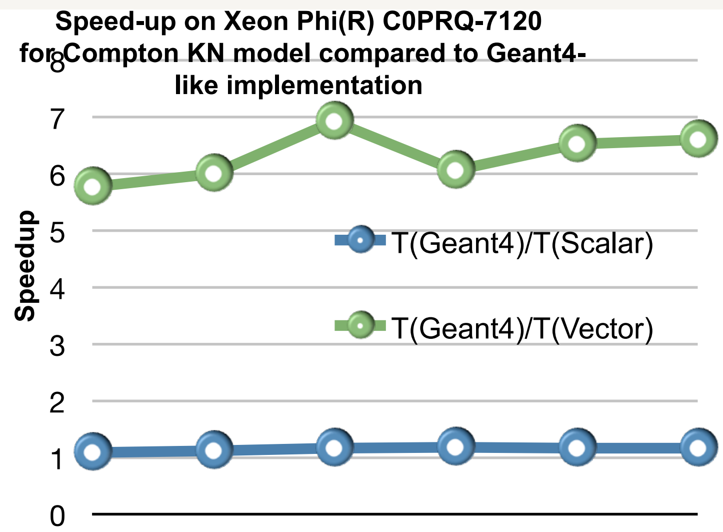
Geometry performance on K20 GPU

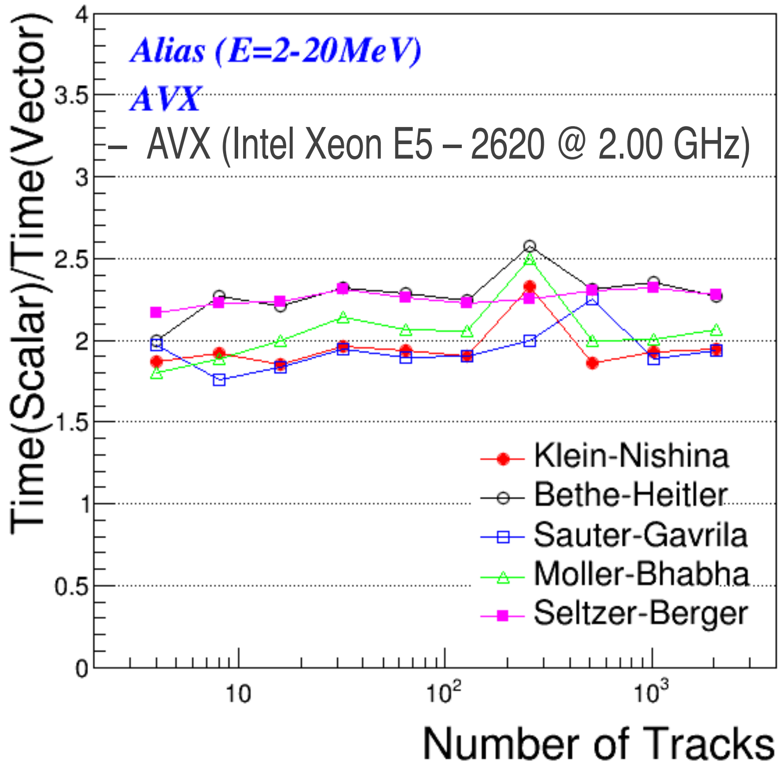
- Speedup for different navigation methods of the box shape, normalized to scalar CPU
  - Scalar (specialized/unspecialized)
  - Vector
  - GPU (Kepler K20)
  - ROOT
- Data transfer in/out is asynchronous
  - Measured only the kernel performance – relying on constant throughput to hide transfer latency
- Will explore how to saturate the die: either with large track containers, running a single kernel, or with smaller containers dynamically scheduled.
- Demonstrates that we can run the same code on CPU/accelerators; further optimization anticipated



Physics

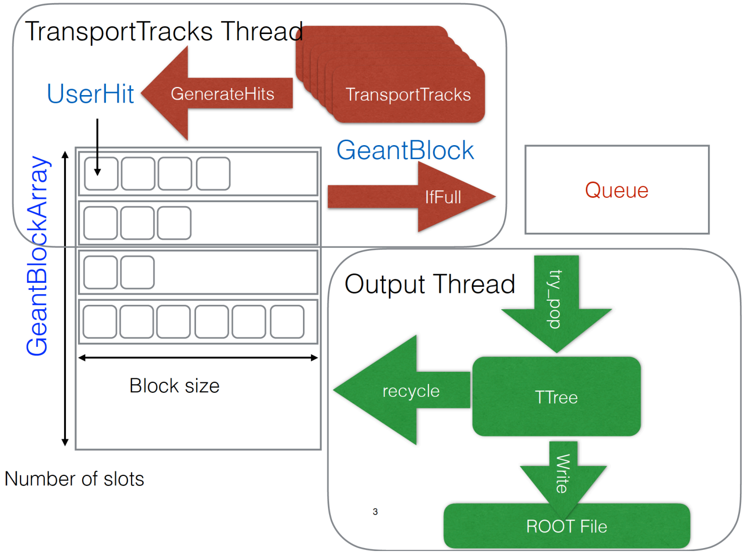
- Objective: a vector/accelerator friendly re-write of physics code
  - Alias sampling (first choice)
  - Accept/reject (when needed)
- Identify when
- The initial vectorized gamma models show performance gain already for small vector size
  - 1.2x – 2.3x on SSE
  - 1.8x – 2.3x on AVX
  - 6x on Xeon Phi
- Use profilers to identify hotspots (vtune, Mac Instruments, igprof)





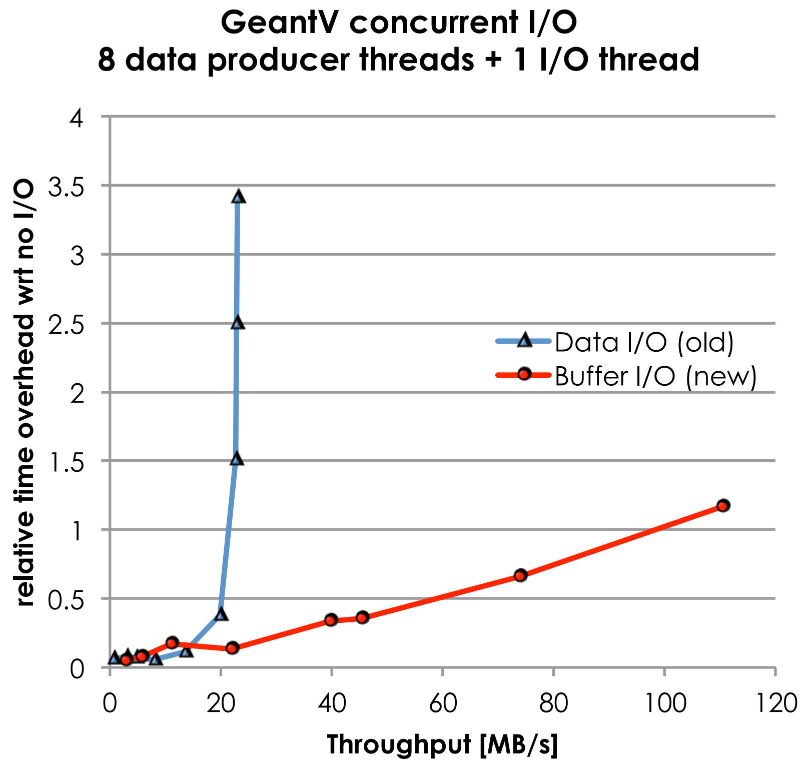
Hits/digits I/O

- "Data" mode
  - Send concurrently data to one thread dealing with full I/O



- "Buffer" mode
  - Send concurrently local trees connected to memory files produced by workers to one thread dealing with merging/write to disk

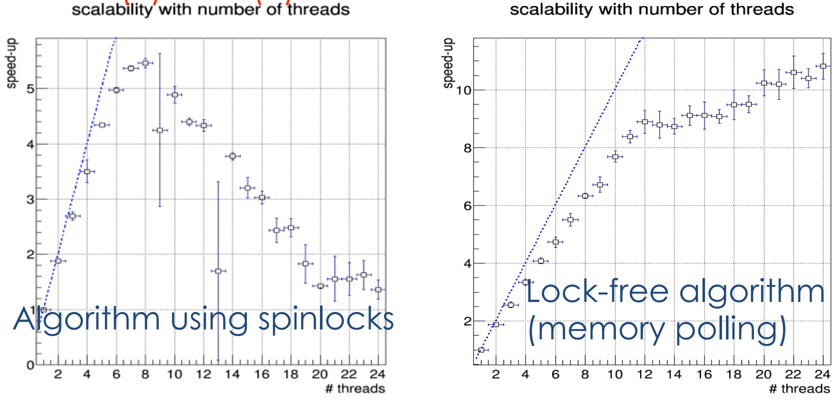
- Integrating user code with a highly concurrent framework should not spoil performance

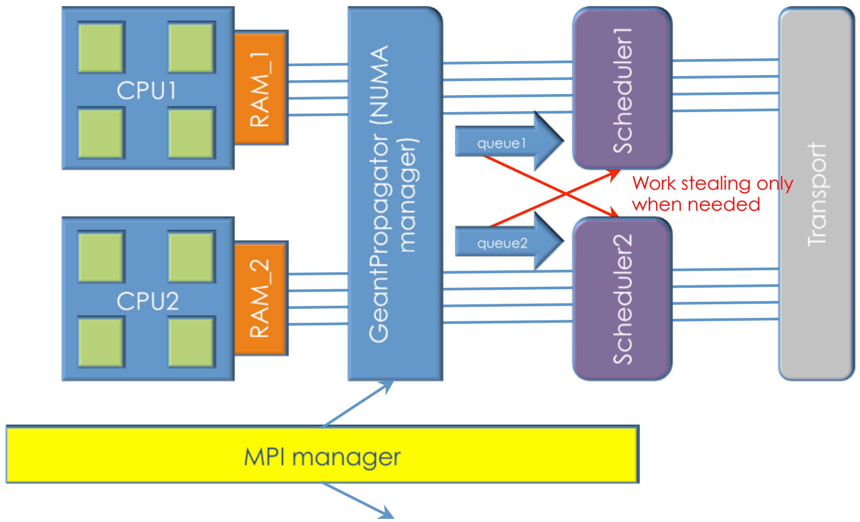


Basketizer performance

- Investigated different ways of scheduling & sharing work - lock free queues, ..
  - Changes in scheduler require non-trivial effort (rewrite)
- Seqerial still large, due to high re-basketizing load (concurrent copying)
  - $O(10^5)$ baskets/second on Intel Core i7™
  - Algorithm already lock free
  - Rate will go down with addition of physics processes
- Ongoing work to improve scalability
  - Re-use baskets for several steps
  - Introduce NUMA awareness
  - Clone scheduler in NUMA-aware groups for use in many cores (e.g. KNL)

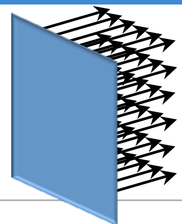
Rebasketizing
2x Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40GHz

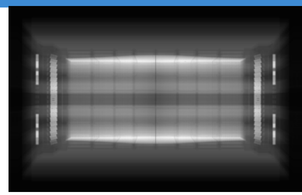


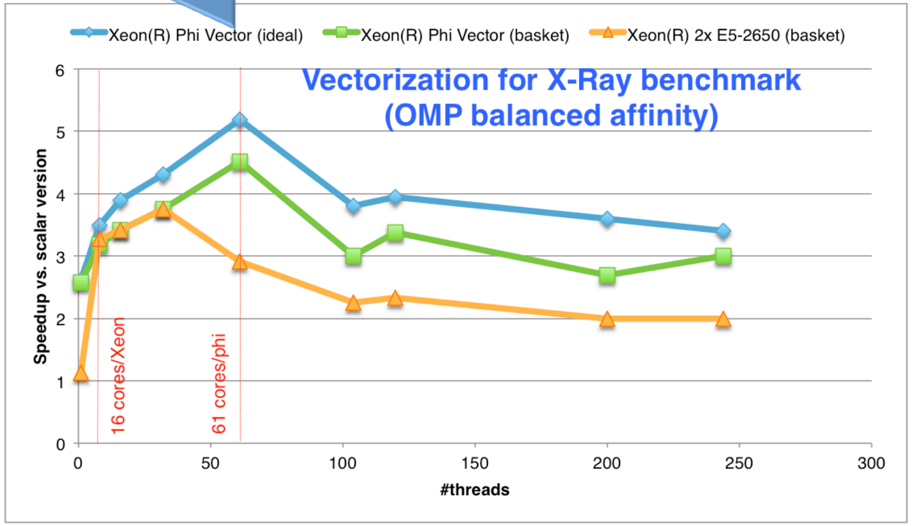


X-ray benchmark: Vector performance

- The X-Ray benchmark tests geometry navigation in a detector geometry
- In simple geometry example (**concentric tubes**) emulates a tracker detector - used for Xeon©Phi benchmark
  - OMP parallelism + "basket" model
- Gained up to 4.5 from vectorization in basketized mode
  - Approaching the ideal case.



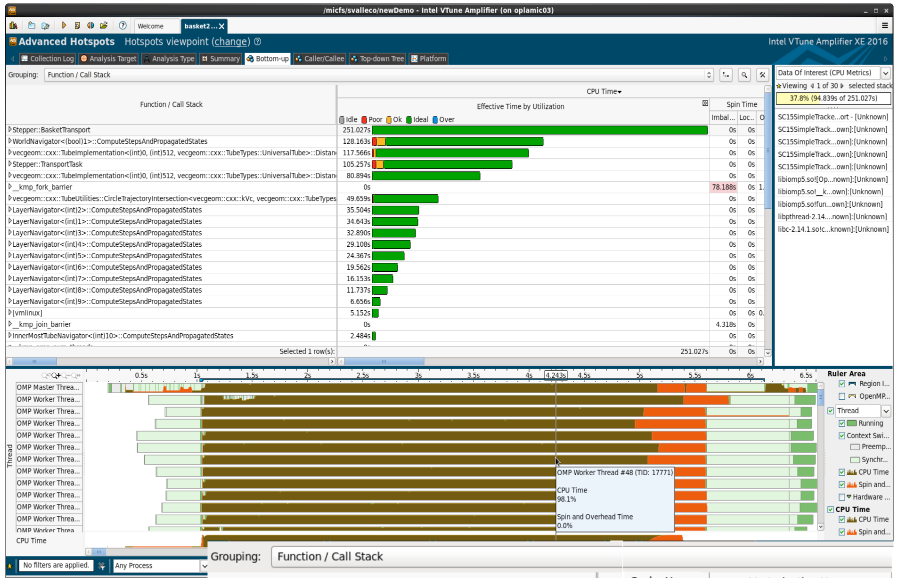


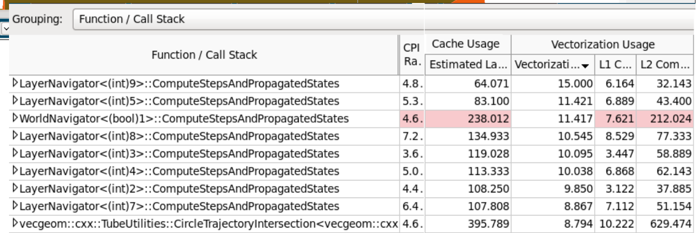


- Scalar case: Simple loop over pixels
- Ideal vectorization case: Fill vectors with N times the same X-ray
- Realistic (basket) case: Group baskets per geometry volume

Profiling for the X-Ray benchmark

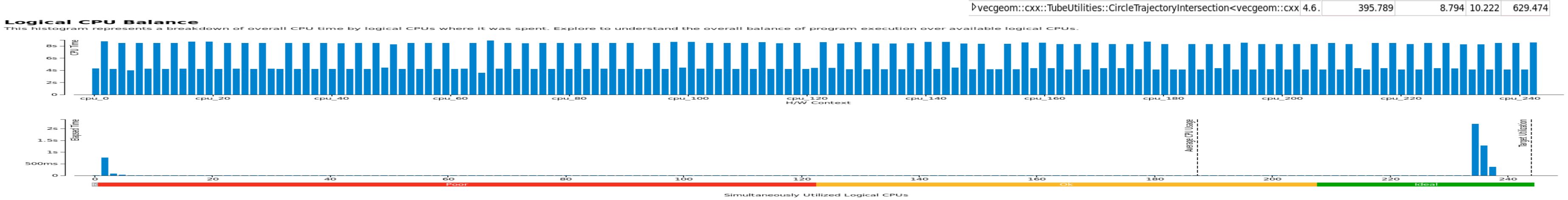
- Good vectorization intensity, thread activity and core usage for the X-Ray basketized benchmark on a Xeon Phi (61 core C0PRQ-7120 P)
- The performance tools gave us good insight on the current performance of GeantV



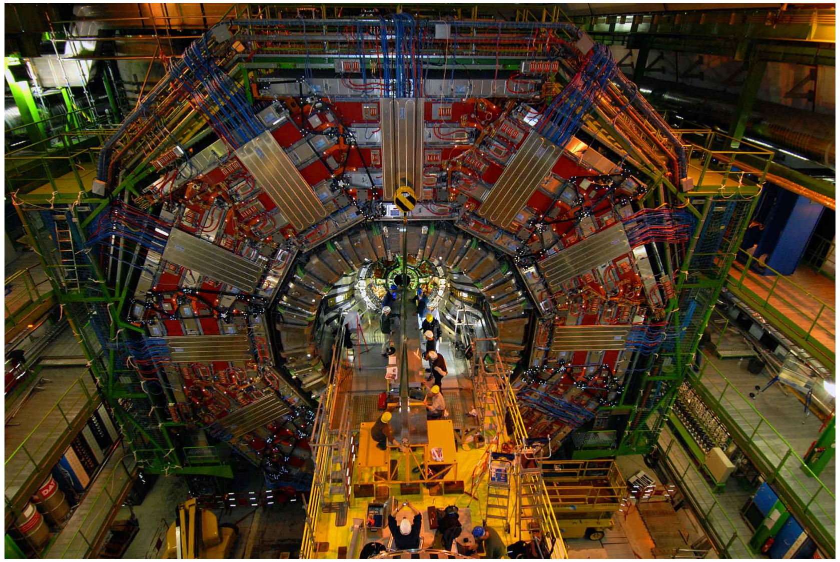


Grouping: Function / Call Stack

Function / Call Stack	CPI Ra.	Cache Usage: Estimated La...	Vectorization Usage: Vectorizati...	L1 C...	L2 Com...
LayerNavigator<(int)9>::ComputeStepsAndPropagatedStates	4.8.	64.071	15.000	6.164	32.143
LayerNavigator<(int)5>::ComputeStepsAndPropagatedStates	5.3.	83.100	11.421	6.889	43.400
WorldNavigator<(bool)1>::ComputeStepsAndPropagatedStates	4.6.	238.012	11.417	7.621	212.024
LayerNavigator<(int)8>::ComputeStepsAndPropagatedStates	7.2.	134.933	10.545	8.529	77.333
LayerNavigator<(int)3>::ComputeStepsAndPropagatedStates	3.6.	119.028	10.095	3.447	58.889
LayerNavigator<(int)4>::ComputeStepsAndPropagatedStates	5.0.	113.333	10.038	6.868	62.143
LayerNavigator<(int)2>::ComputeStepsAndPropagatedStates	4.4.	108.250	9.850	3.122	37.885
LayerNavigator<(int)7>::ComputeStepsAndPropagatedStates	6.4.	107.808	8.867	7.112	51.154
vecgeom::cxx::TubeUtilities::CircleTrajectoryIntersection<vecgeom::cxx	4.6.	395.789	8.794	10.222	629.474



Putting It All Together - CMS Yardstick



- Some of the improvements can be back ported to G4
- Overhead of basket handling is under control
- Ready to take advantage of vectorization throughout.

Improvement Factors (total) with respect to G4

Legacy (TGeo) Geometry library:

- **1.5** → Algorithmic improvements in infrastructure.

2015 VecGeom (estimate)

- **2.4** → Algorithmic improvements in Geometry

Upcoming VecGeom (early result)

- **3.3** → Further Geometric algorithmic improvements and some vectorization

Summary

- GeantV is in development mode – and in many cases researching different approaches or techniques
- A significant performance gain is a raison d'etre of GeantV
- Benchmarking of individual classes is constantly done
- Benchmarks of simple setups are created to monitor, understand and improve the performance of new components
- Profilers are key tools in performance improvement

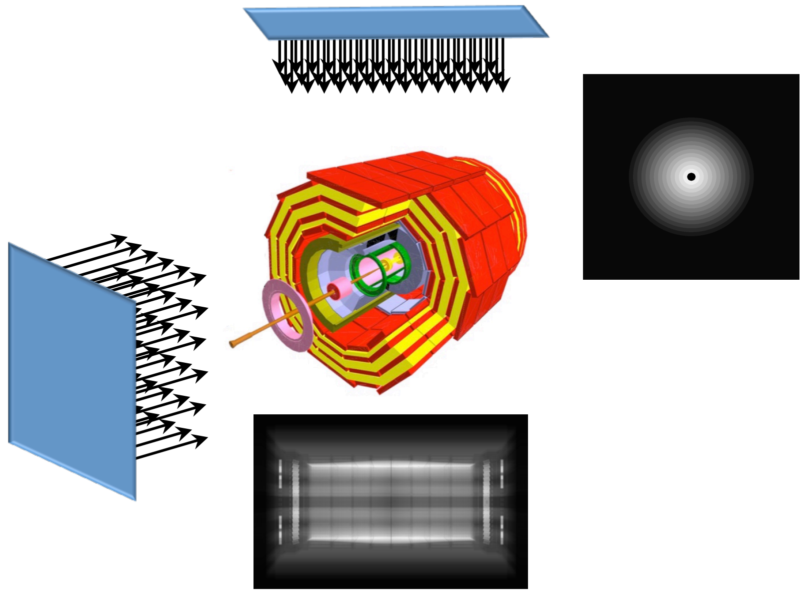
The authors acknowledge the contribution and support from

- Intel (funding, technical and expert advisory, SW/HW)
- CERN openlab

Thank you!

The X-Ray benchmark

- The X-Ray benchmark tests geometry navigation in a real detector geometry
- *X-Ray* scans a module with virtual rays in a grid corresponding to pixels on the final image
  - Each ray is propagated from boundary to boundary
  - Pixel gray level determined by number of crossings
- A simple geometry example (concentric tubes) emulating a tracker detector used for Xeon©Phi benchmark
  - To probe the vectorized geometry elements + global navigation as task
  - OMP parallelism + “basket” model

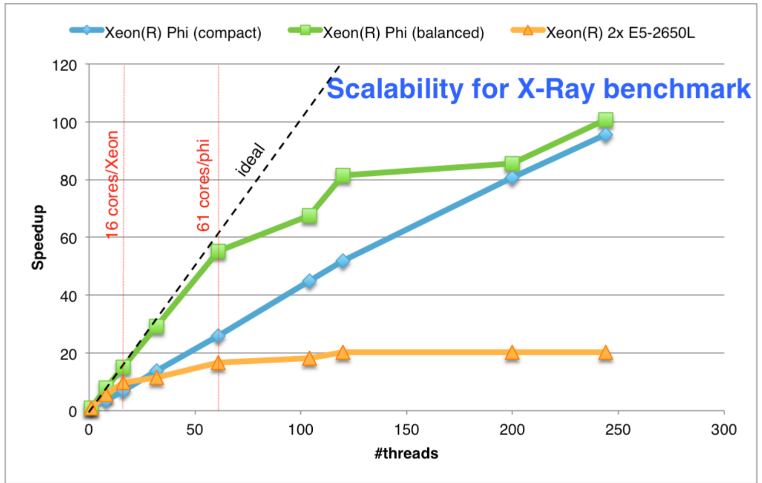


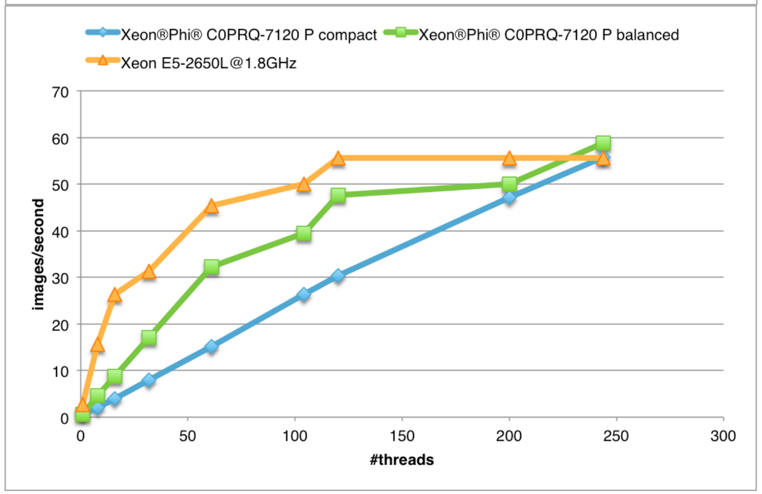
Scalability and throughput

- Better behavior using OMP balanced
  - Approaching well the ideal curve up to native cores count
  - Balanced threading converges towards the compact model as all the thread slots are filled

- It's worth to run Xeon Phi saturated for our application

- The throughput performance for a saturated KNC is equivalent (for this setup) to the dual Xeon E5-2650L@1.8GHz server which hosts the card.



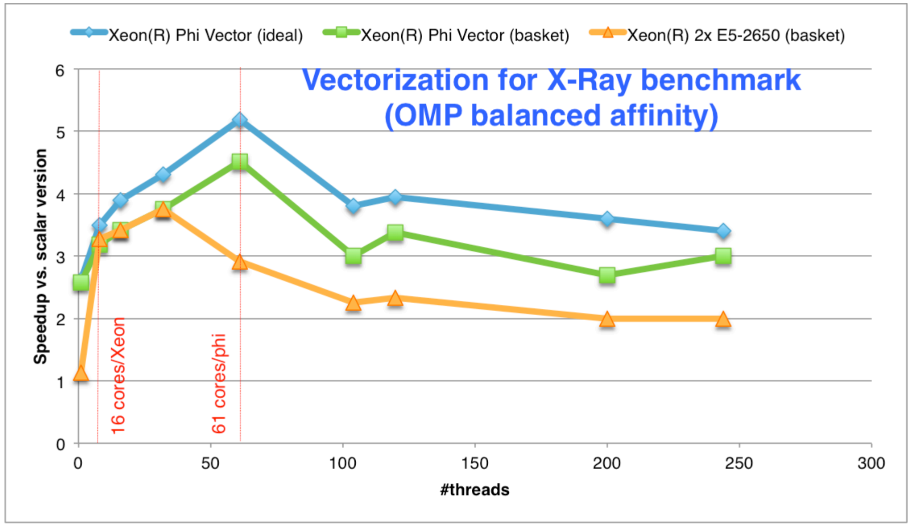


Next steps

- Repeat the test with the introduction of
  - Vectorised EM physics
  - Vectorised transport in Mag Field
- Develop simple classes for materials and particles to be able to run on coprocessors to enable physics on the GPU and Xeon Phi full CMS yardstick
- … implementing a "preliminary performance yard-stick" combining all prototype features
  - SIMD gains in the full CMS experiment setup
  - Coprocessor broker in action: part of the full transport kernel running on Xeon®Phi® and GPGPU
  - Scalability and NUMA awareness for rebasketizing procedure
  - … achieving these just moves the target a bit further
- … testing scaling up to large node count through MPI, e.g. on CORI
  - Input distribution and Output gathering.

Vector performance

- Gaining up to 4.5 from vectorization in basketized mode
  - Approaching the ideal vectorization case (when no regrouping of vectors is done) .
- Vector starvation starts when filling more thread slots than the core count
  - Performance loss is not dramatic
  - Better vectorization compared to the Sandy-Bridge host (expected)



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