The path toward High Performance Computing in High Energy Physics

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THE GEANTV PROJECT

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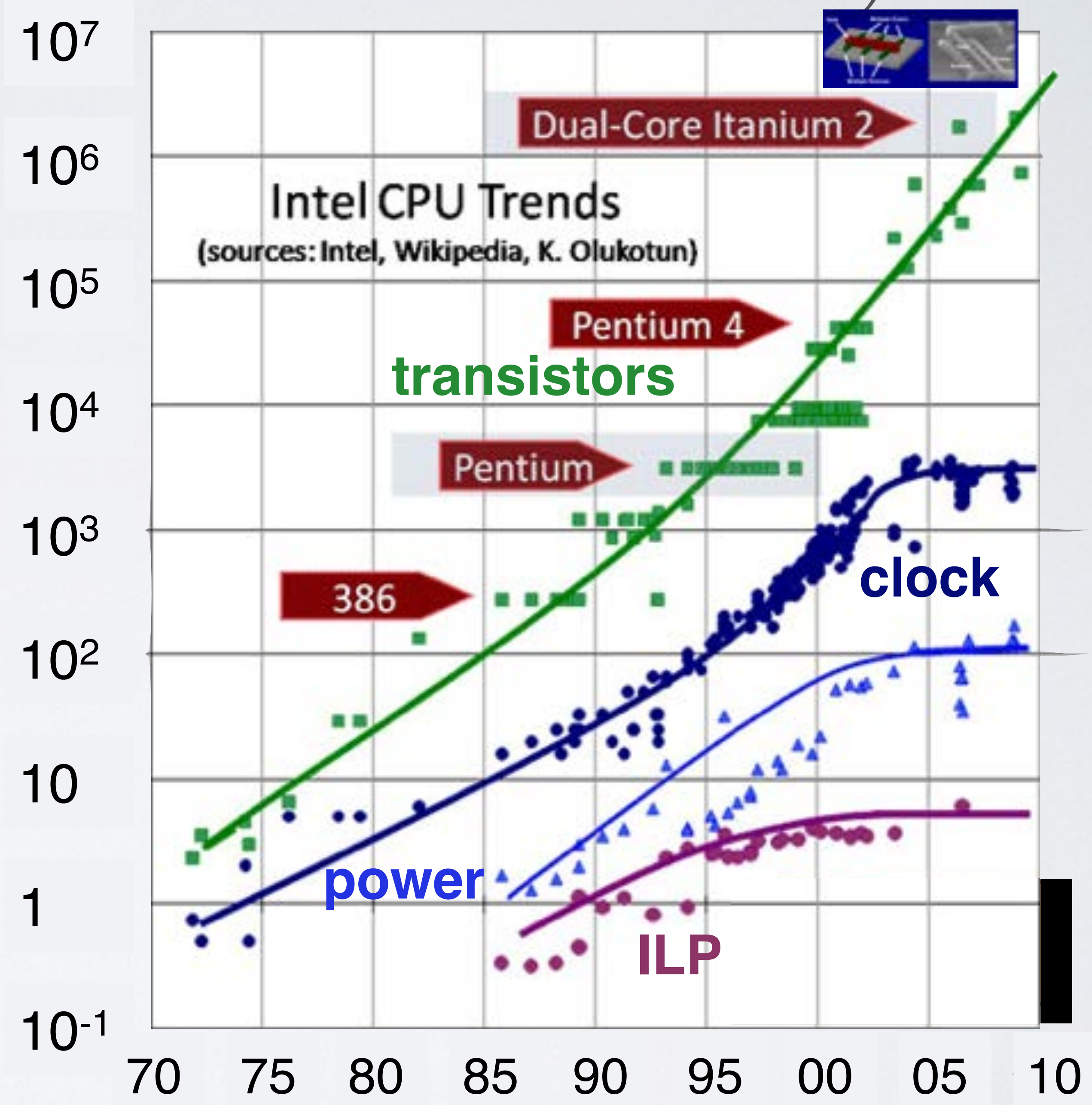
WHY DO WE NEED HPC?

- WLCG
  - 170 computing centres in 42 countries
  - ~500k Cores
  - O(200) PB on disk

MOTIVATIONS

(EVEN IF YOU ARE FAMILIAR WITH THEM)

- Performance of our code almost stagnant
- SIMD is key to achieve the performance we need (10x)
- Portability, better physics and optimisation will be the targets
- Simulation
    - 50% of the LWGC cycles
    - can show how to better exploit CPUs for complex applications



THE EIGHT DIMENSIONS

- The "dimensions of performance"
  - Vectors
  - Instruction Pipelining
  - Instruction Level Parallelism (ILP)
  - Hardware threading
  - Clock frequency
  - Multi-core
  - Multi-socket
  - Multi-node

Micro-parallelism: gain in throughput and in time-to-solution

Very little gain to be expected and no action to be taken

Gain in memory footprint and time-to-solution but not in throughput

Possibly running different jobs as we do now is the best solution

Expected limits on performance scaling

	SIMD	ILP	HW
THEORY	8	4	1.35
OPTIMISED	6	1.57	1.25
HEP	1	0.8	1.25

Expected limits on performance scaling (multiplied)

	SIMD	ILP	HW
THEORY	8	32	43.2
OPTIMISED	6	9.43	11.79
HEP	1	0.8	1

OpenLab@CHEP12

WHY IT IS SO DIFFICULT?

- No clear kernel
- C++XX code generation / optimisation not well understood
- Most of the technology is coming out now
  - Lack of standards
  - Technological risk
- Non professional coders
- Fast evolving code
- No control on hardware acquisition

WHY SIMULATION?

- Simulation can be developed in a "system independent" way
- It can be prototyped with "little I/O" (at the beginning)
- The LHC experiments use extensively G4 as main simulation engine. They have invested in validation procedures
- Experiments develop their own fast MC solution as a full simulation is too slow for several physics analysis
- We need an architecture where fast and full MC can be run together with the highest performance on parallel systems

WHY GEANTV?

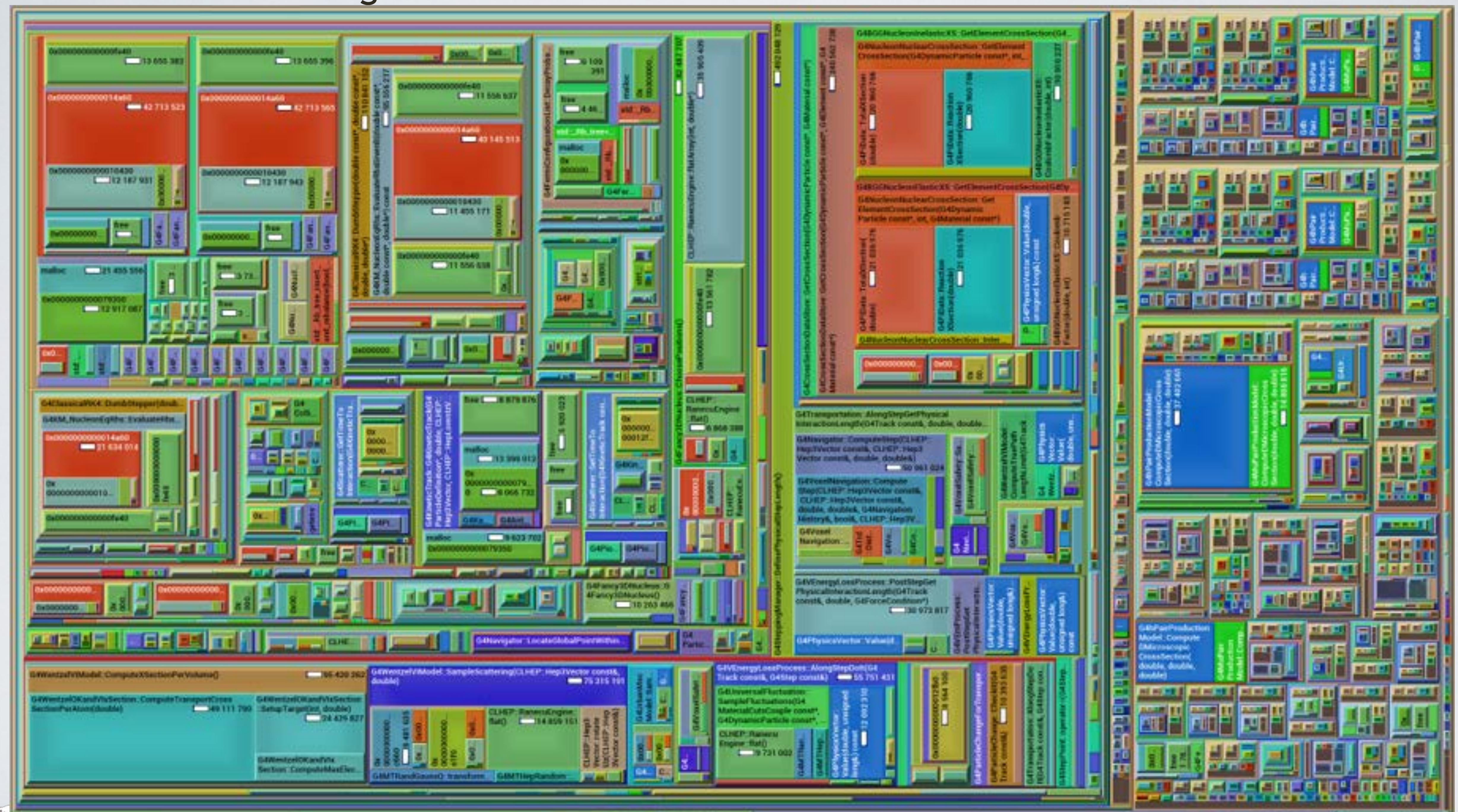
- Simulation is largely experiment independent
- Geant4 is THE simulation code for HEP
- 50% of the WLCG cycles are used by simulation

WHY NOT GEANT4+?

- Extensive prototyping and analysis has convinced us that "vectorisation" of Geant4 was not achievable without a major rewrite of the code
  - No hotspots (!)
  - Virtual table structure very deep and complex (1990's style)
  - Codebase very large and non-homogeneous
- No criticism, but even the best things age

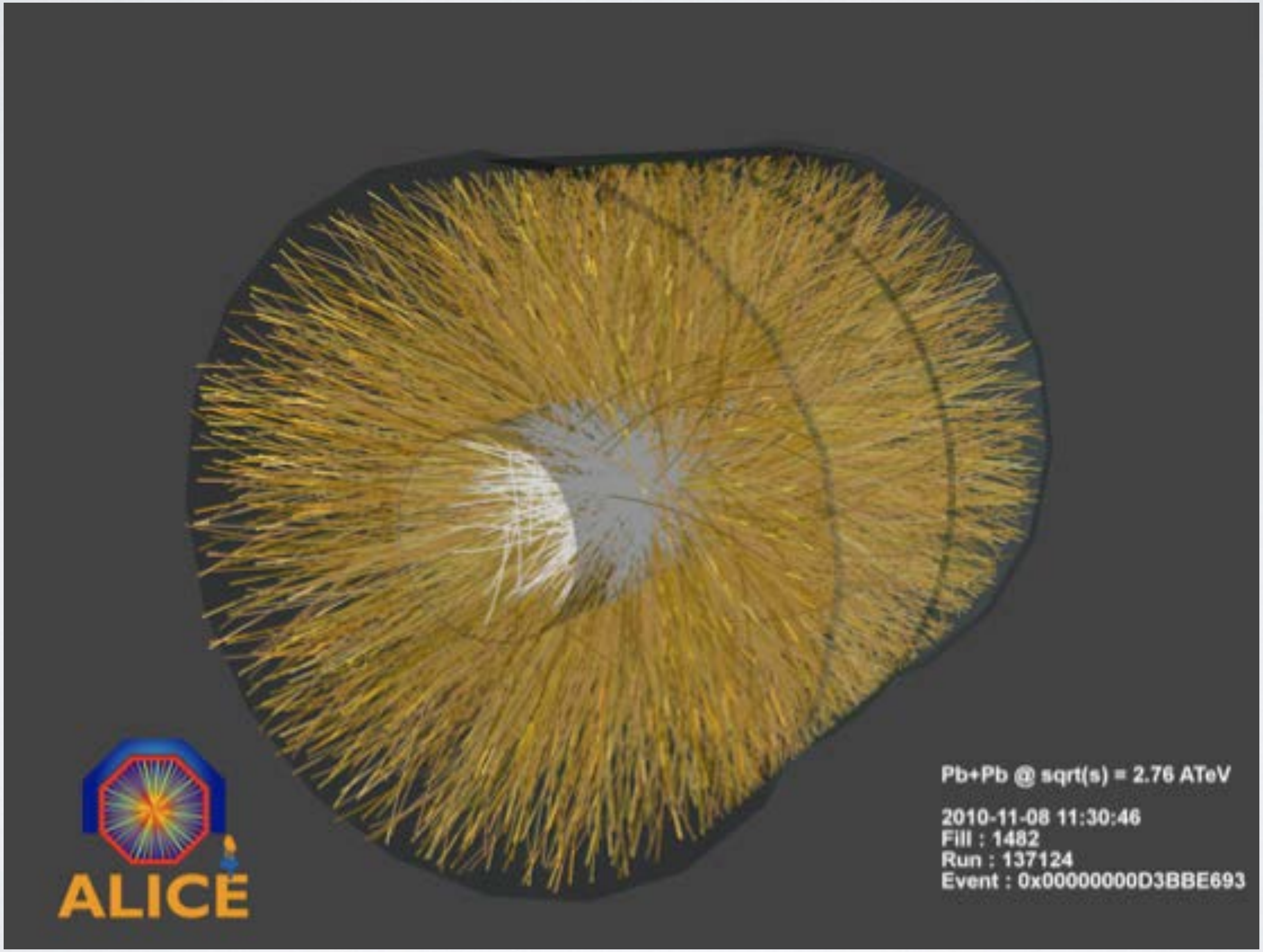
GEANT4 PROFILING EXAMPLE: CALL MAP

valgrind / kcachegrind



Anything above 10% is a pathology!

PARALLELISM EVERYWHERE AGAIN… BUT HOW TO EXPLOIT IT?

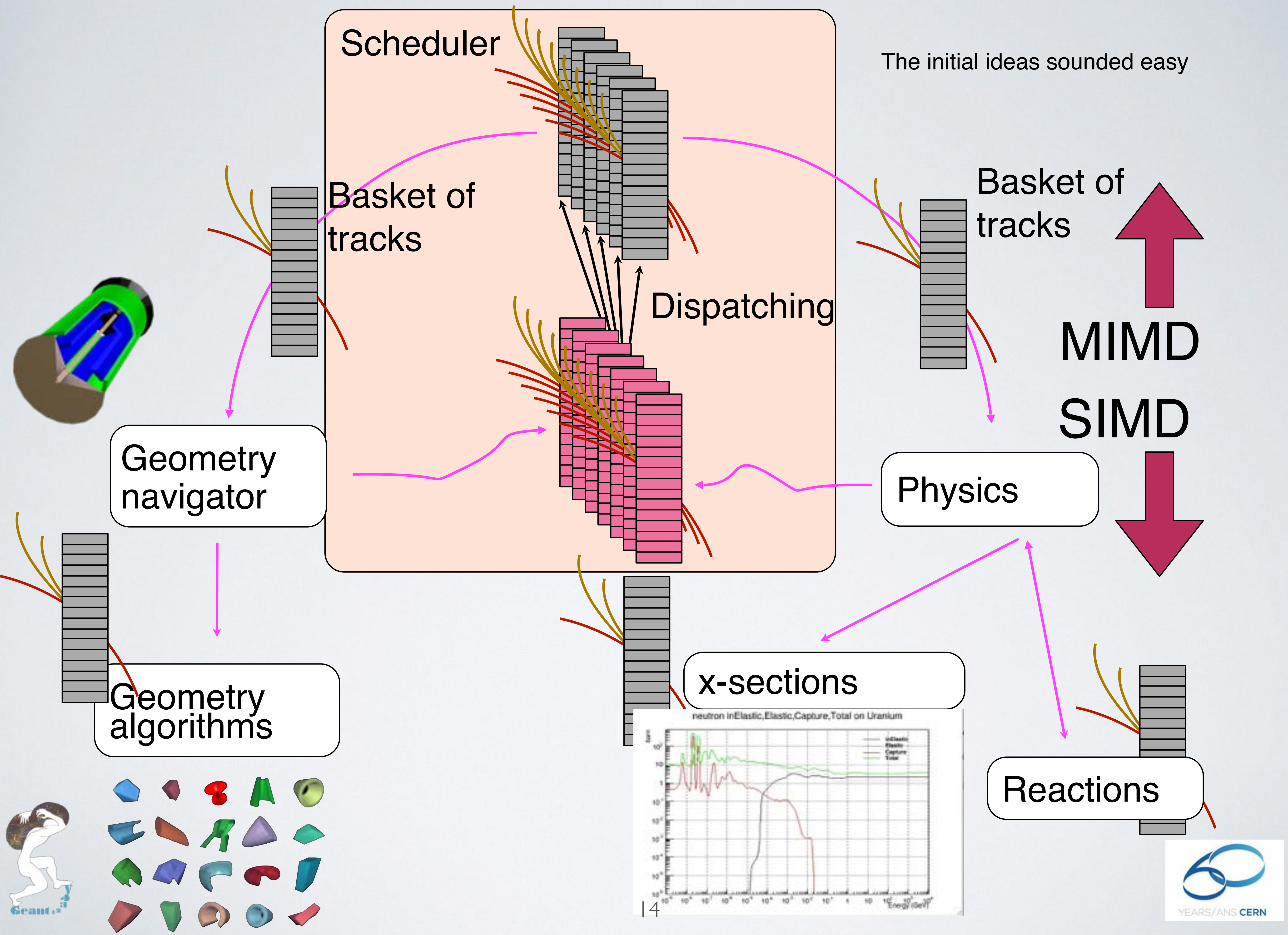


?

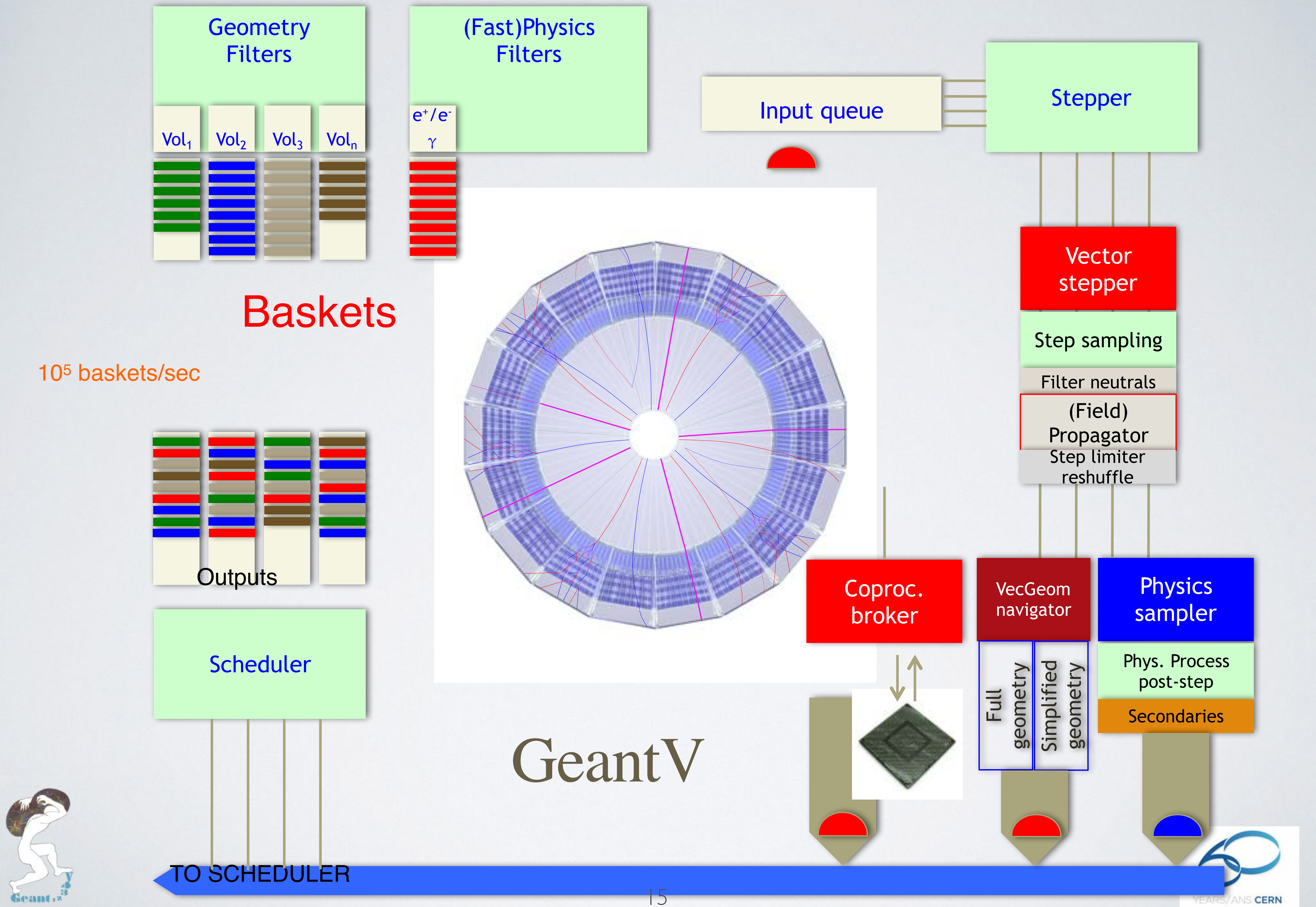
In some sense… but not entirely
(see later)

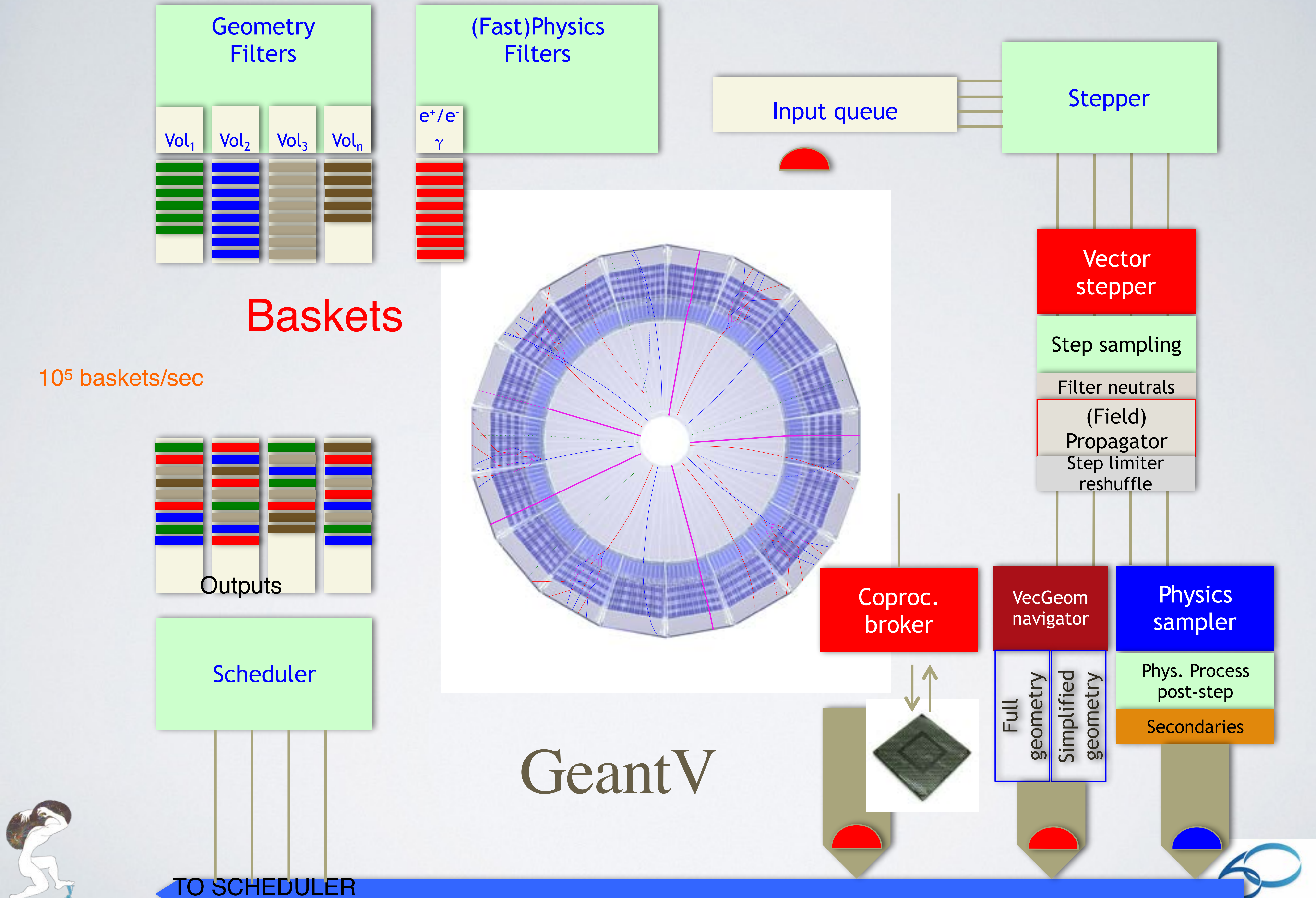
WHAT DO WE WANT TO DO?

- Develop an all-particle transport simulation programme with
  - A code 2-5 times faster than Geant4
  - Continue improvement of physics
  - Full simulation and various fast simulation options
  - Portable on different architectures (CPUs, GPUs and Xeon Phi's)
- Understand the limiting factors for a (10x) improvement



The initial ideas sounded easy
Scheduler
Basket of tracks
Basket of tracks
Dispatching
MIMD
SIMD
Geometry navigator
Physics
Geometry algorithms
x-sections
neutron inElastic,Elastic,Capture,Total on Uranium
Reactions


Geometry Filters
Vol$_1$
Vol$_2$
Vol$_3$
Vol$_n$
(Fast)Physics Filters
e^+/e^-
γ
Input queue
Stepper
Baskets
10^5 baskets/sec
Vector stepper
Step sampling
Filter neutrals
(Field) Propagator
Step limiter reshuffle
Outputs
Scheduler
Coproc. broker
VecGeom navigator
Physics sampler
Full geometry
Simplified geometry
Phys. Process post-step
Secondaries
GeantV
TO SCHEDULER


Geometry Filters
Vol1
Vol2
Vol3
Voln
(Fast)Physics Filters
e+/e-
γ
Input queue
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Baskets
10⁵ baskets/sec
Vector stepper
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Filter neutrals
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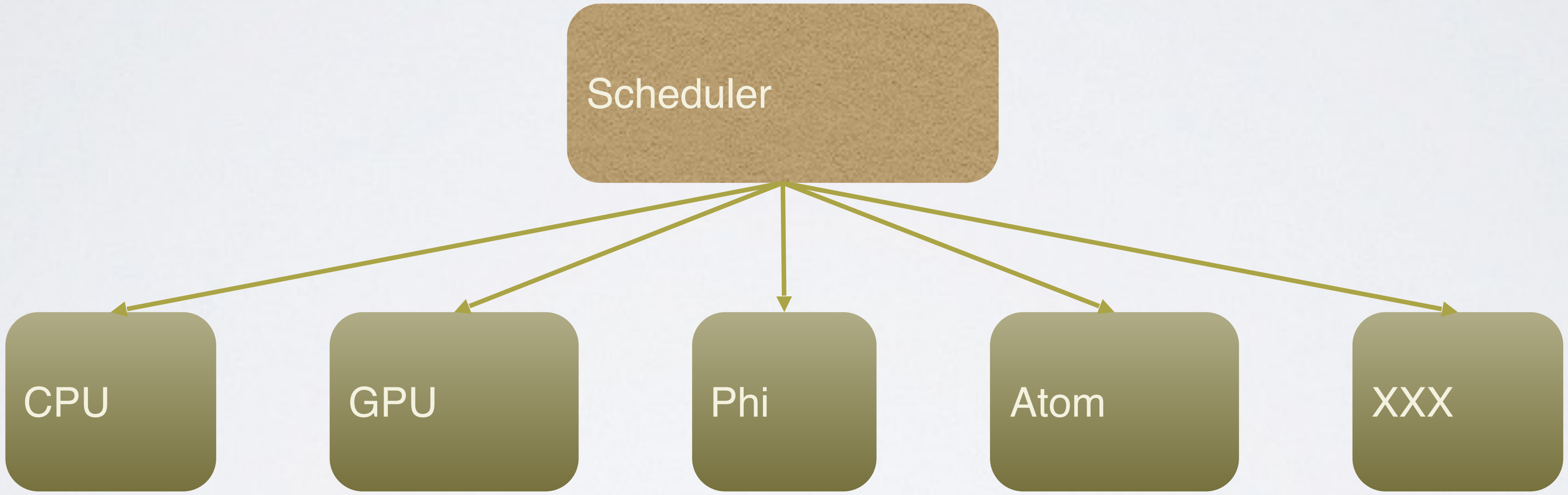
TO SCHEDULER

CHALLENGES

- Overhead from reshuffling particle lists should not offset SIMD gains
- Exploit the metal at its best, while maintaining portability



- Test from the onset on a "large" setup (LHC-like detector)
  - Toy models tell us very little – complexity is the problem

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

PORTABILITY

- Long-term maintainability of the code => write one single version of each algorithm and to specialise it to the platform via template programming and low level optimised libraries (Vc in our case)
- A Xeon Phi specific backend is being developed
- Results are quite encouraging: maybe portable HPC is NOT an oxymoron after all…

Here how

“Backend” is a (trait) struct encapsulating standard types/properties for “scalar, vector, CUDA” programming; makes information injection into template function easy

1 particle API

Many particle API (SIMD)

Common C++ template functions

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

```
Vc::double_v distance( Vc::double_v );
```

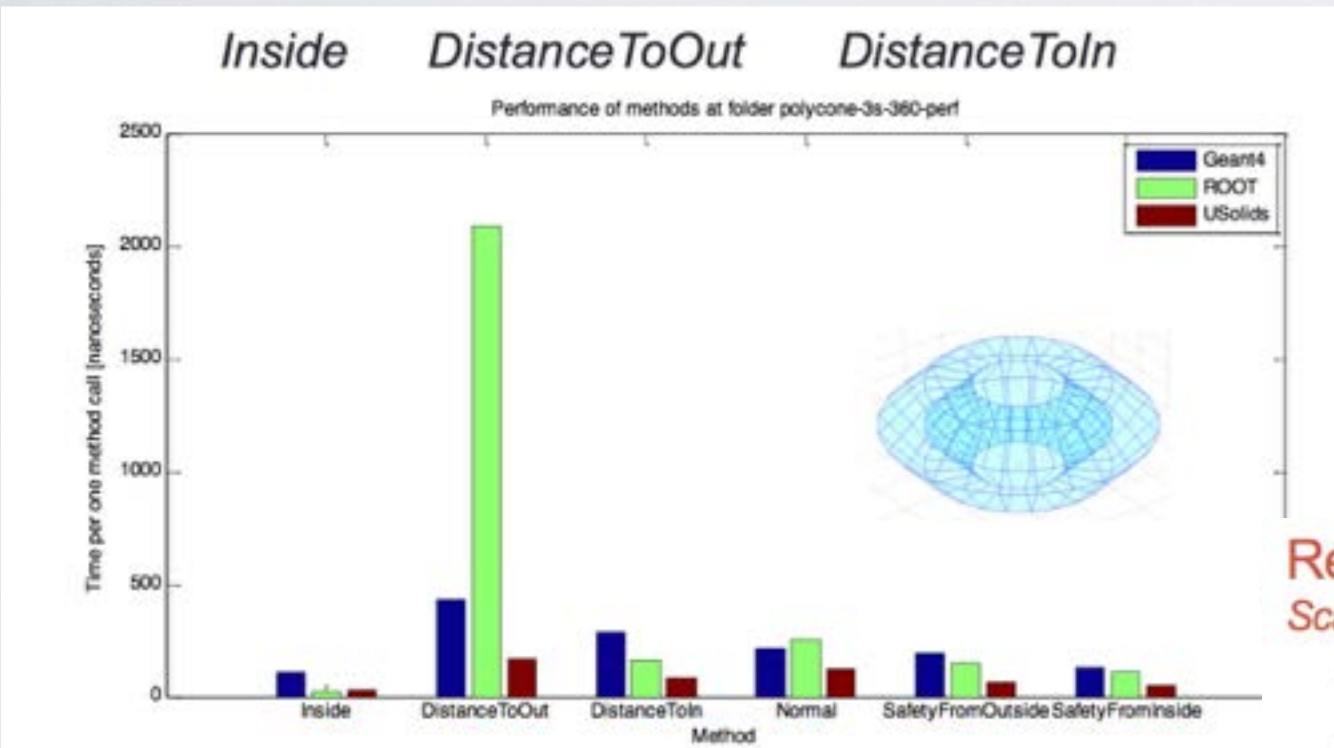
```
template<class Backend>
Backend::double_t
common_distance_function( Backend::double_t input
)
{
   // Algorithm using Backend types
}
```

```
struct ScalarBackend
{
   typedef double double_t;
   typedef bool   bool_t;
   static const bool IsScalar=true;
   static const bool IsSIMD=false;
};
```

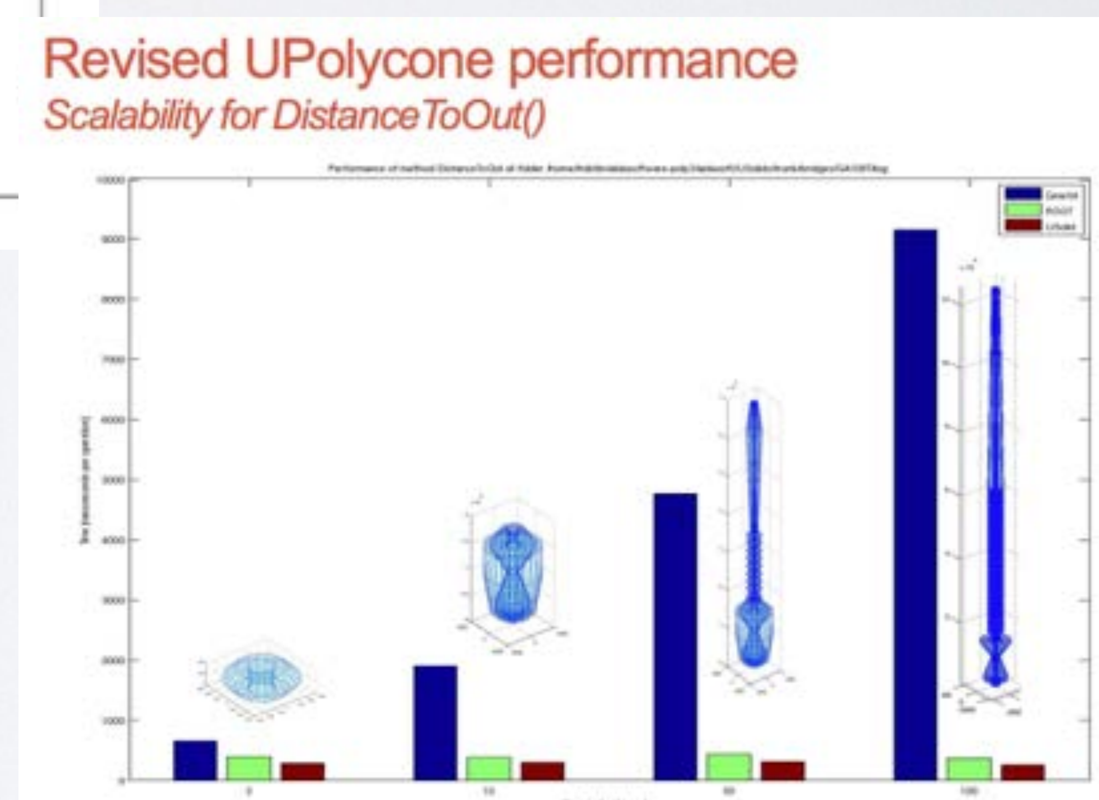
```
struct VectorBackend
{
   typedef Vc::double_v double_t;
   typedef Vc::bool_v bool_t;
   static const bool IsScalar=false;
   static const bool IsSIMD=true;
};
```

ANOTHER EXAMPLE POLYCONE

Speedup factor **3.3x** vs. Geant4, **7.6x** vs. Root • for most performance critical methods, i.e.:



- It is today possible to run Geant4 simulations with USolids shapes replacing Geant4 shapes (seamless to user)
- Geant4 10.1. ships USolids internally optionally one may also compile against external USolids installation



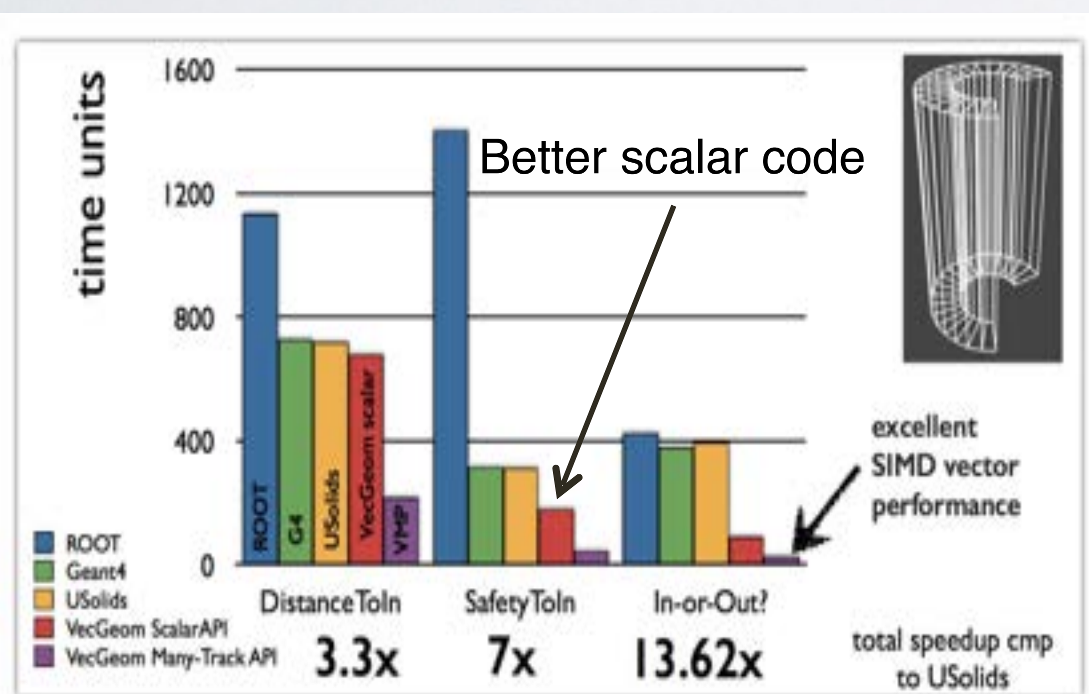
- USolids source code repository: gitlab.cern.ch/VecGeom/VecGeom

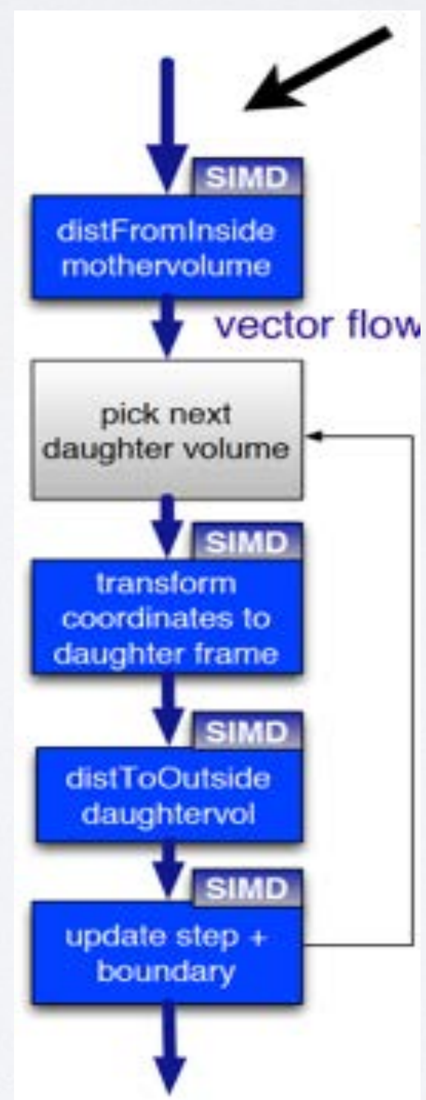
Ugeom/VecGeom is developed by the AIDA project.

GEOMETRY PERFORMANCE (PHI VS XEON)

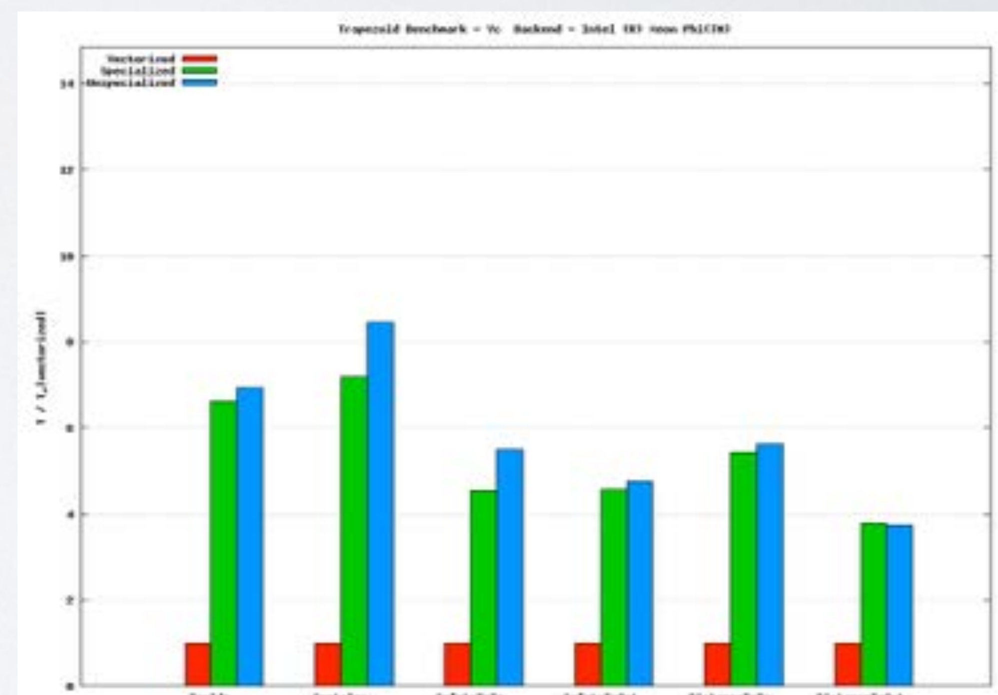
- Geometry is 30-40% of the total CPU time in Geant4
- A library of vectorized geometry algorithms to take maximum advantage of SIMD architectures
- Substantial performance gains also in scalar mode
- Testing the same on on GPU

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





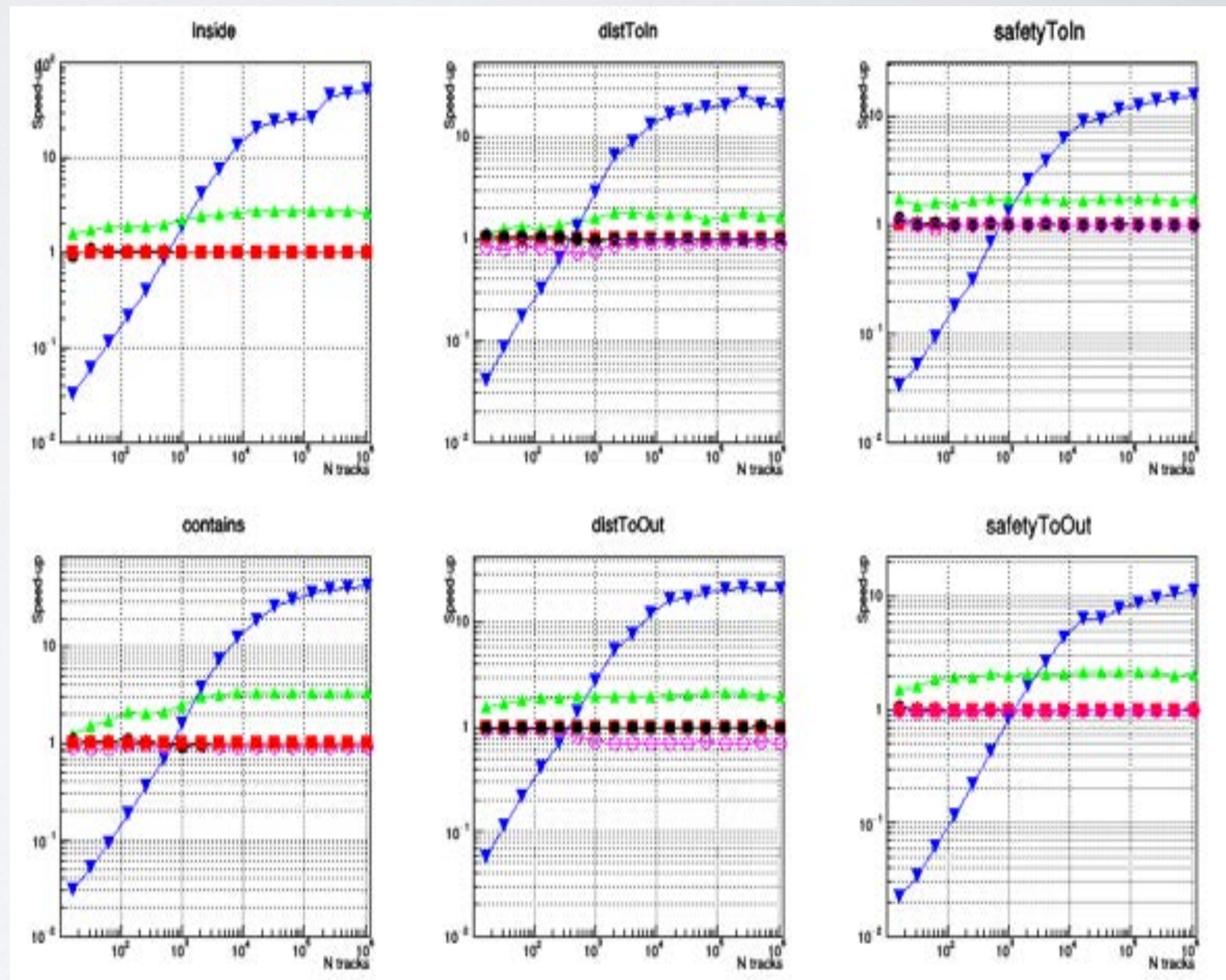
Overall performance for a simplified detector vs. scalar ROOT/5.34.17



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

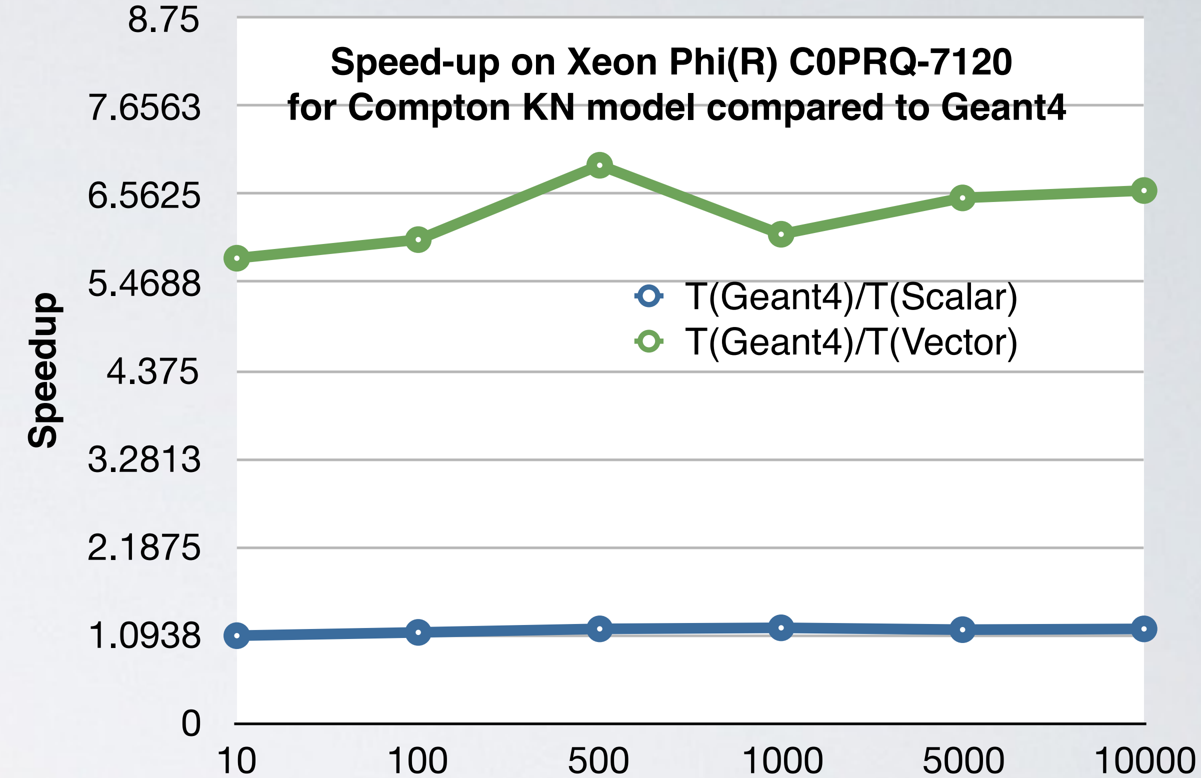
GEOMETRY PERFORMANCE ON K20

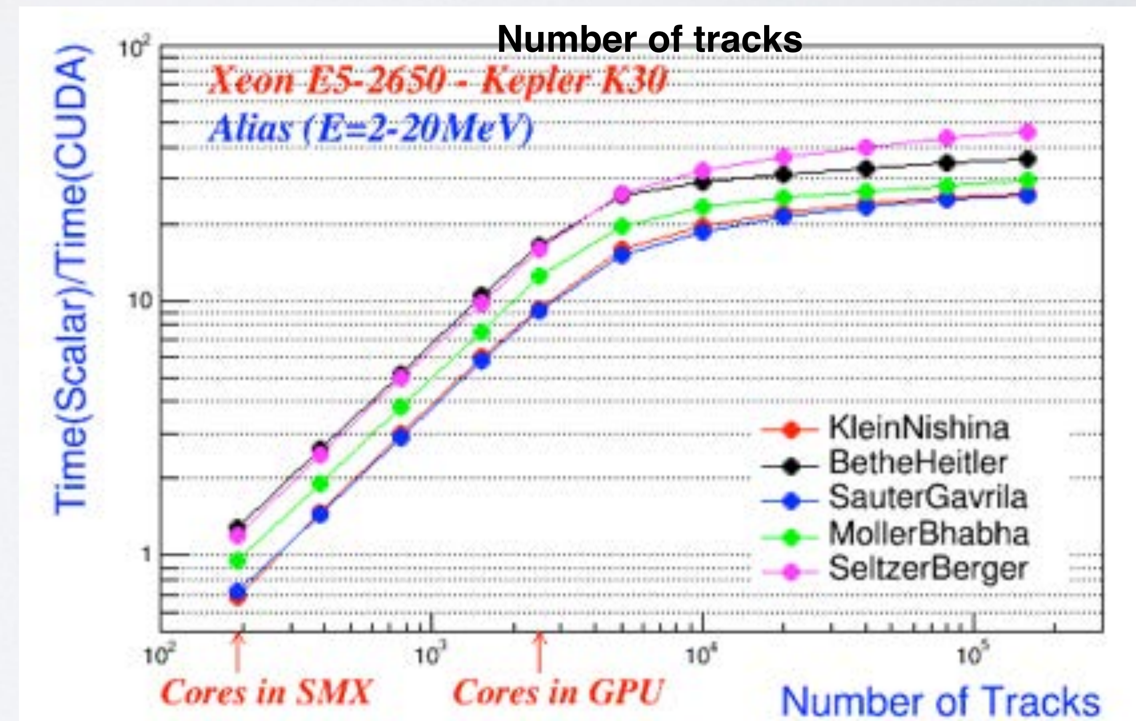
- Speedup for different navigation methods of the box shape, normalized to scalar CPU
  - Scalar (specialized/unspecialized)
  - Vector
  - GPU (Kepler K20)
  - ROOT
- Data transfer in/out is asynchronous
  - Measured only the kernel performance, but providing constant throughput can hide transfer latency
- The die can be saturated with both large track containers, running a single kernel, or with smaller containers dynamically scheduled.
- Just a baseline proving we can run the same code on CPU/accelerators, to be optimized



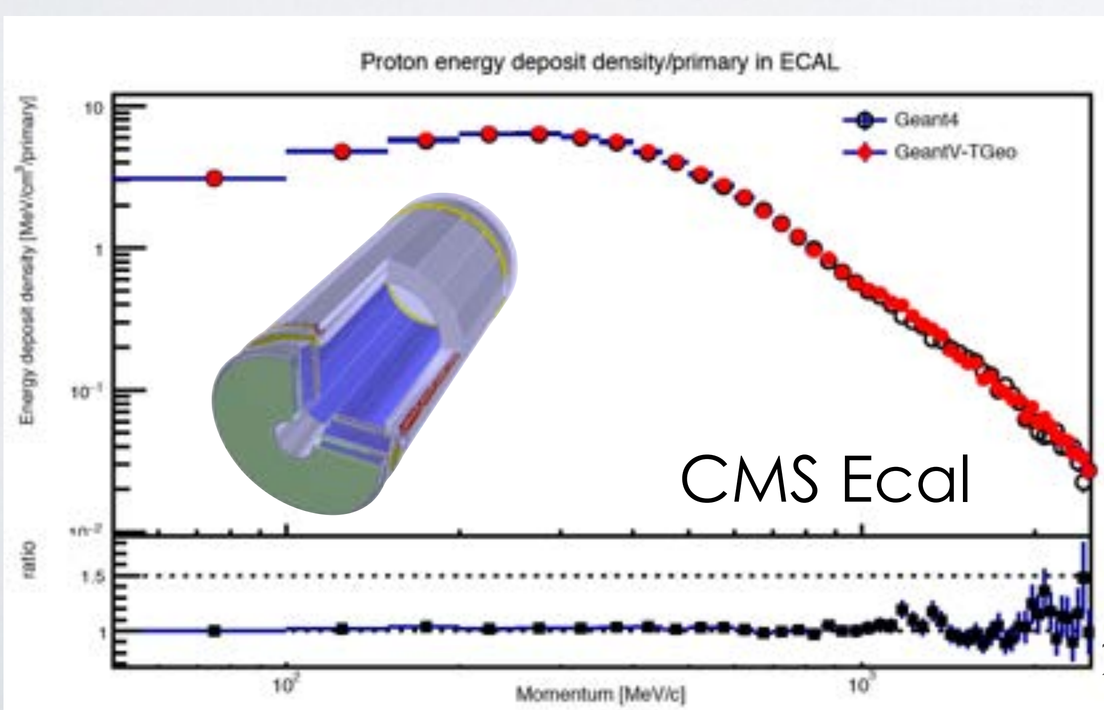
PHYSICS PERFORMANCE

- Objective: a vector/accelerator friendly re-write of physics code
- The vectorised Compton scattering shows good performance gains
- Current prototype able to run an exercise at the scale of an LHC experiment (CMS)
    - Simplified (tabulated) physics but full geometry, RK propagator in field
    - **Preliminary results hint to performance improvements of 3-4**



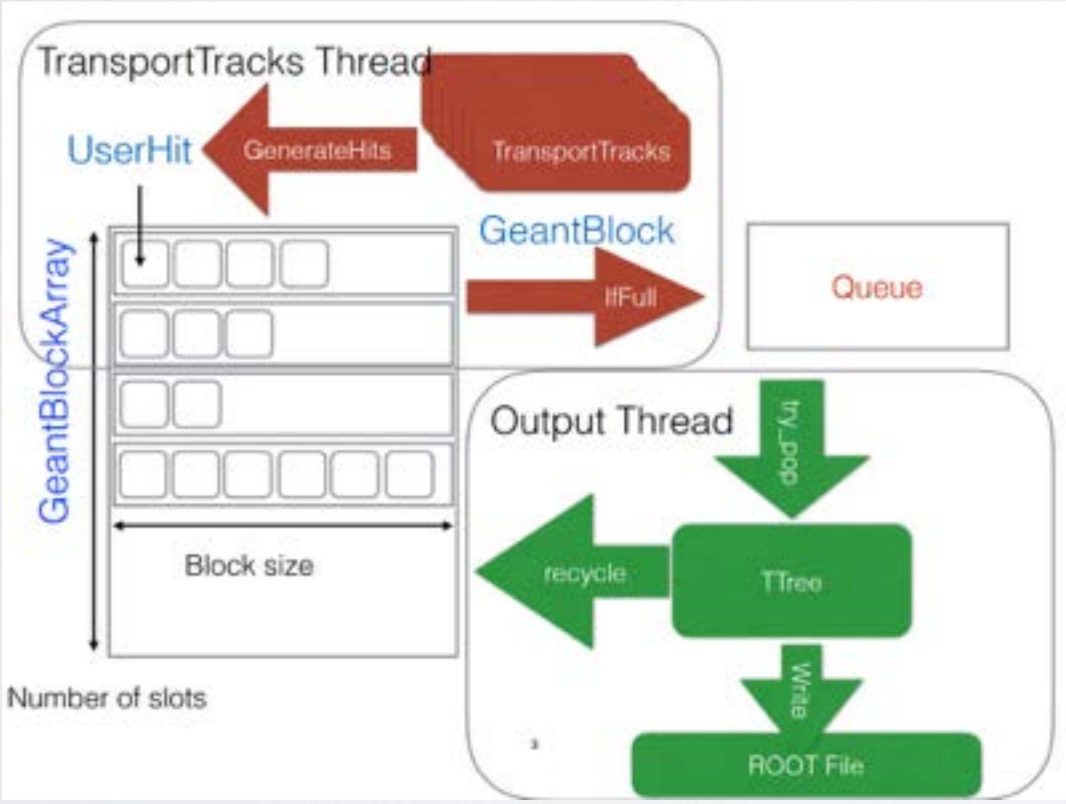


Alias sampling performance on a Kepler K30 (Soon' Y. - EM physics models on parallel computing architectures)



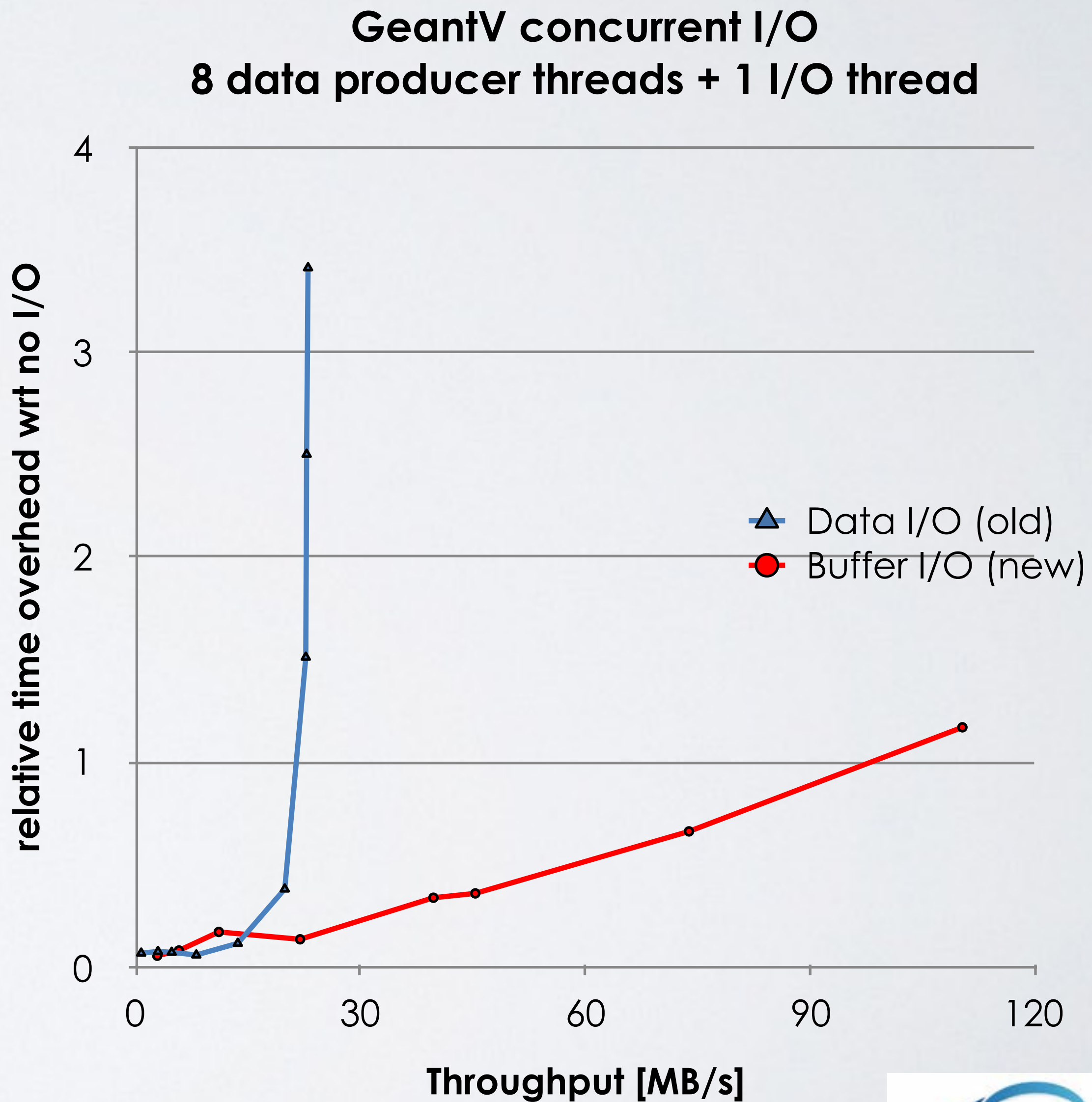
HITS/DIGITS I/O

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



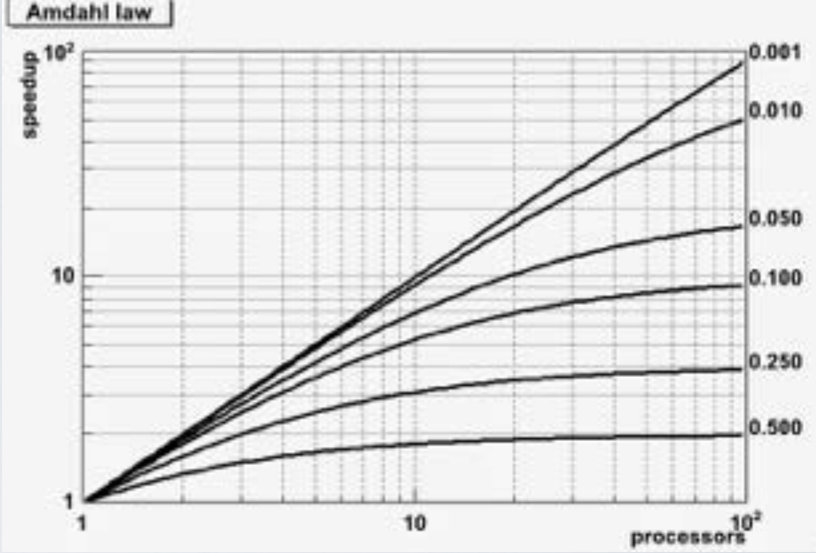
- "Buffer" mode
  - Send concurrently local trees connected to memory files produced by workers to one thread dealing with merging/write to disk

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

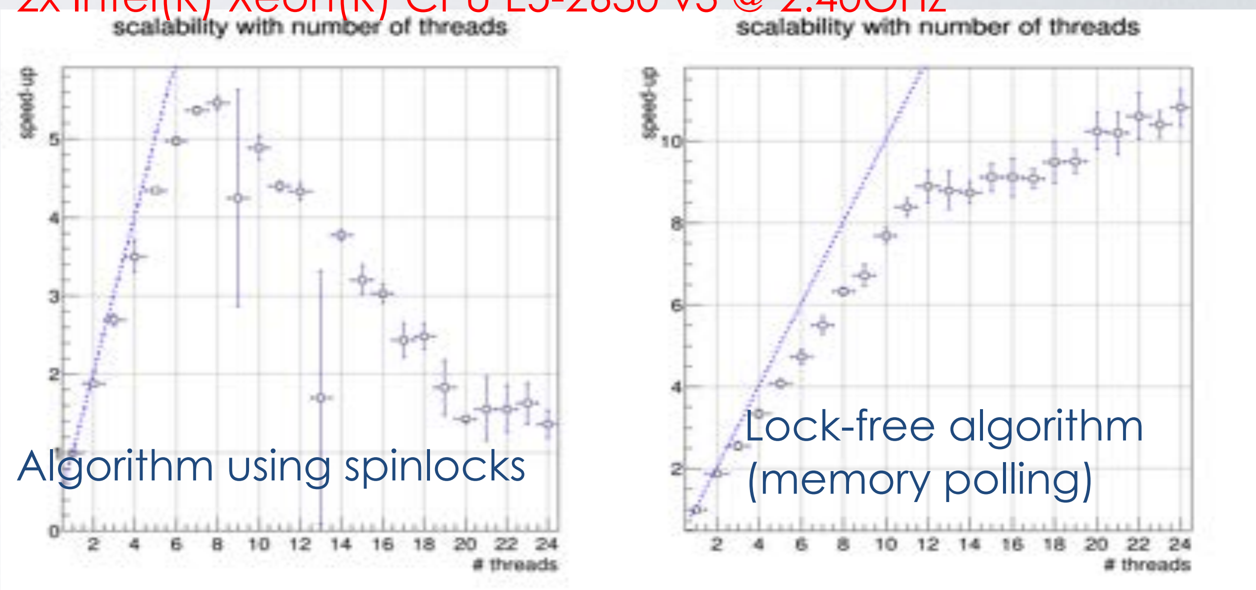


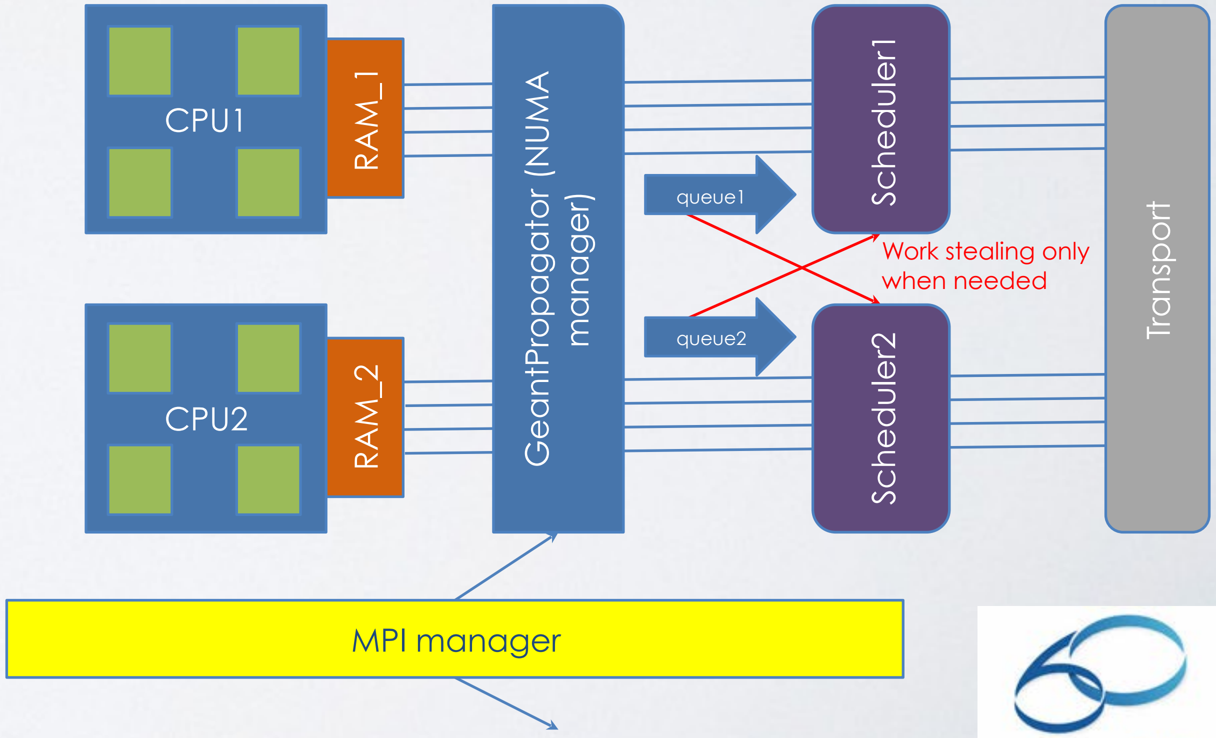
BASKETIZER PERFORMANCE

- Investigated different ways of scheduling & sharing work - lock free queues, ..
  - Changes in scheduler require non-trivial effort (rewrite)
- Amdahl 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 physics processes
- Ongoing work to improve scalability
  - Re-use baskets in the same thread after step if enough particles doing physics-limited steps
  - Clone scheduling in NUMA aware groups, important for many cores (e.g. KNL)

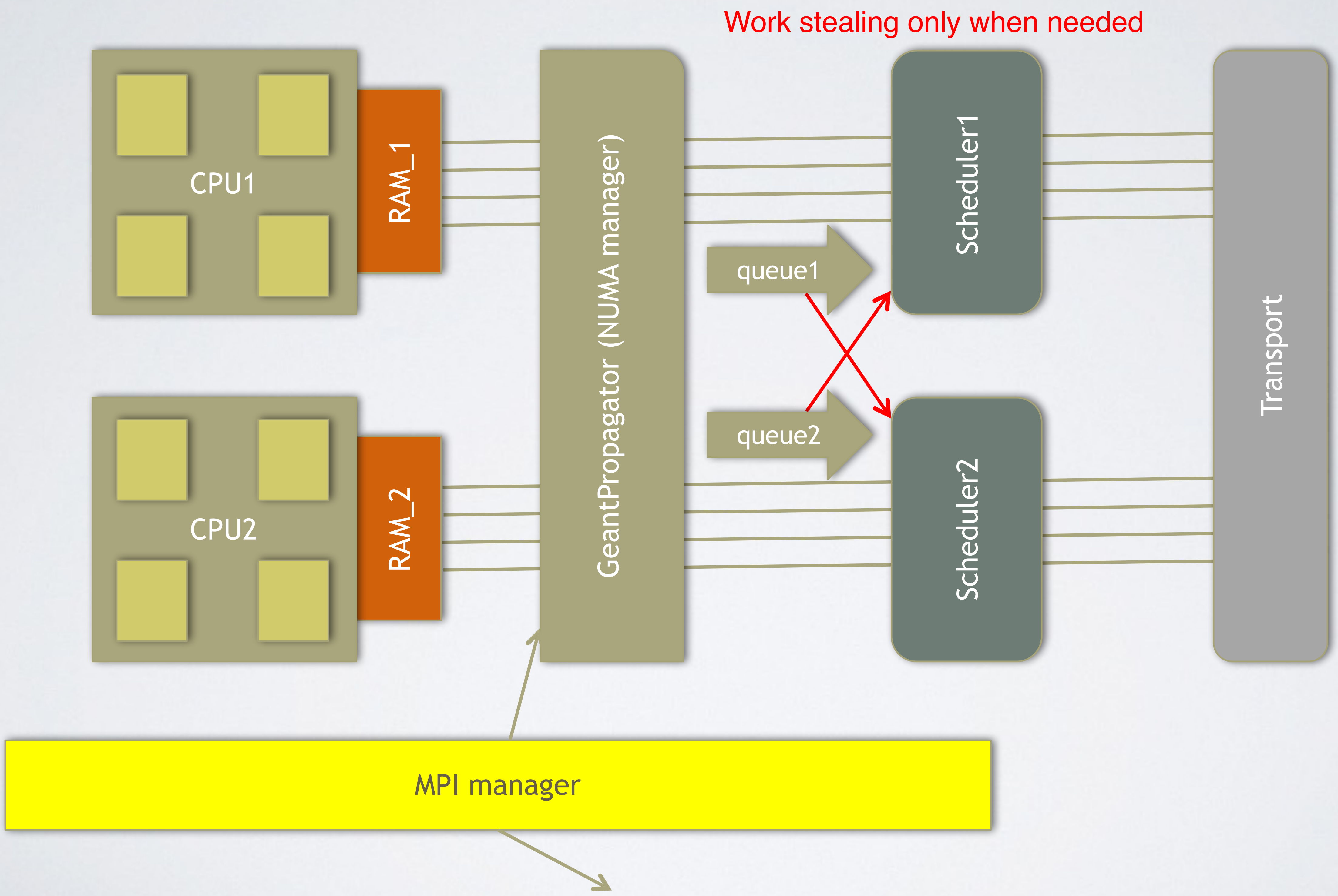


Rebasketizing
2x Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40GHz



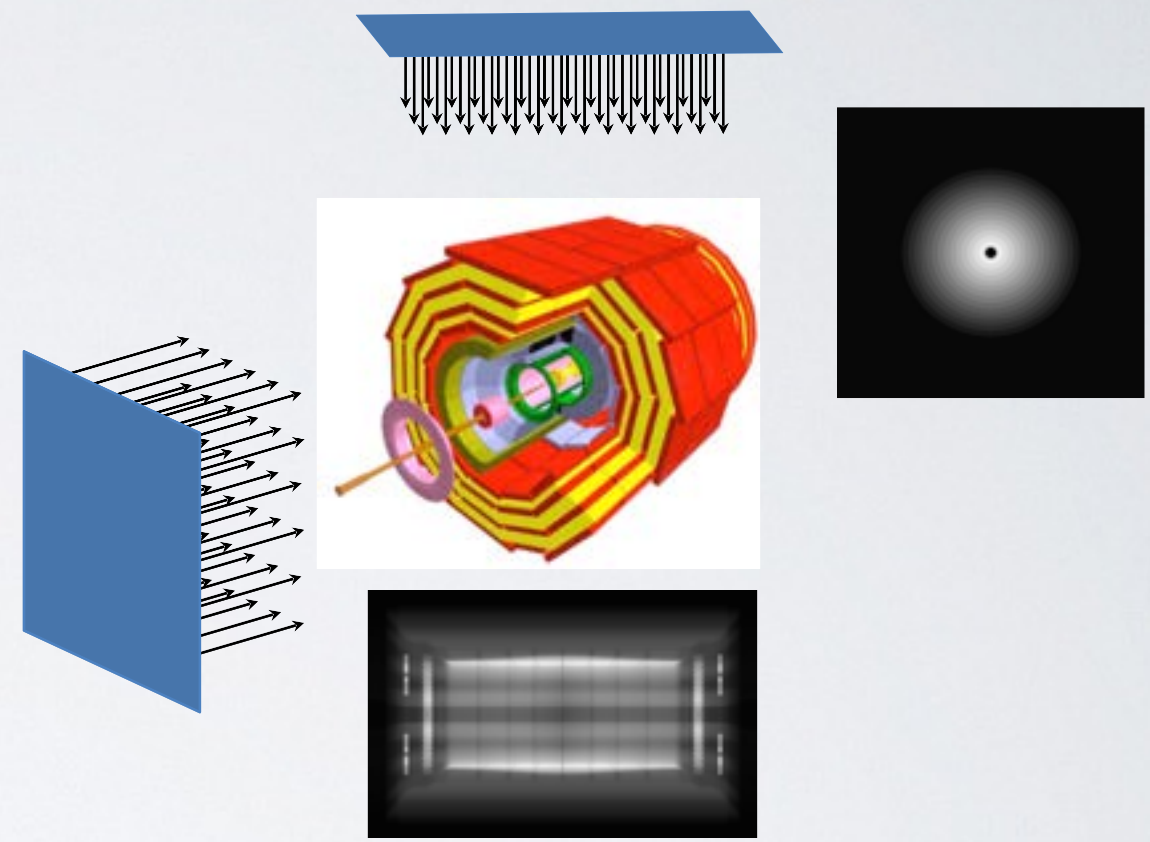


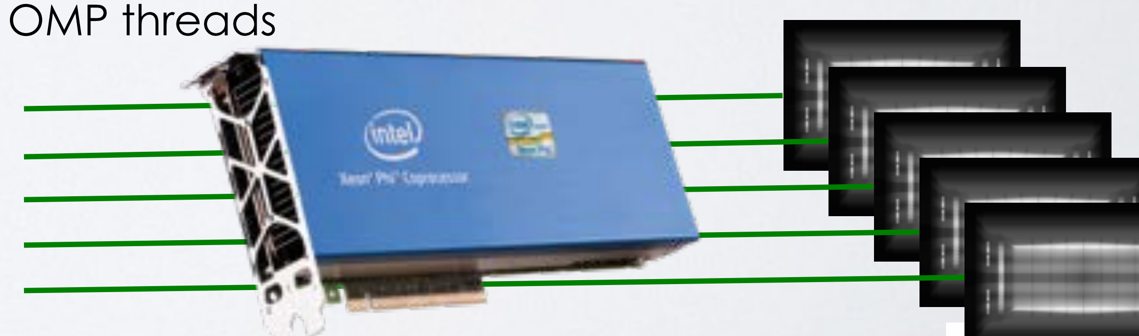
"CLONING" THE SCHEDULER



THE X-RAY BENCHMARK

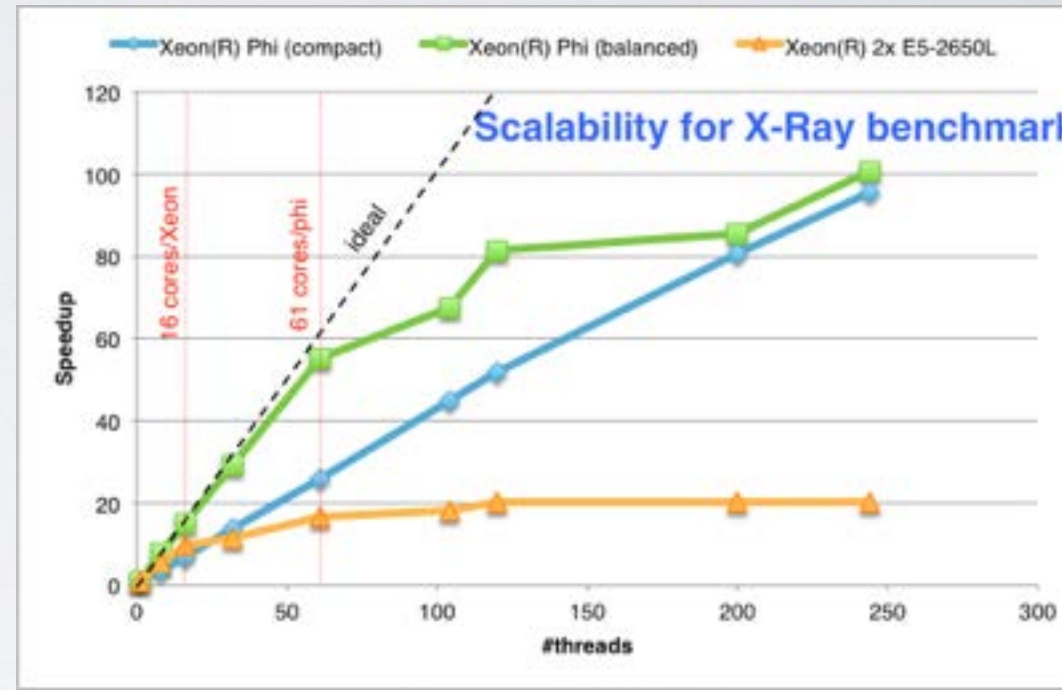
- The X-Ray benchmark tests geometry navigation in a real detector geometry
- *X-Ray* scans a module with virtual rays in a grid corresponding to pixels on the final image
  - Each ray is propagated from boundary to boundary
  - Pixel gray level determined by number of crossings
- A simple geometry example (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

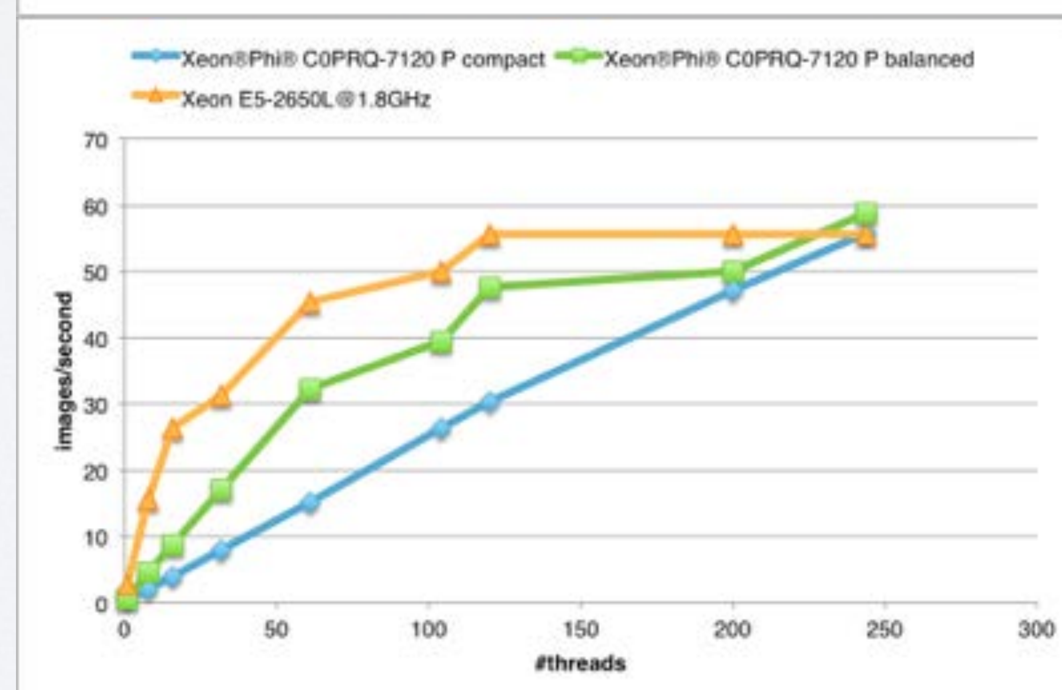




SCALABILITY AND THROUGHPUT

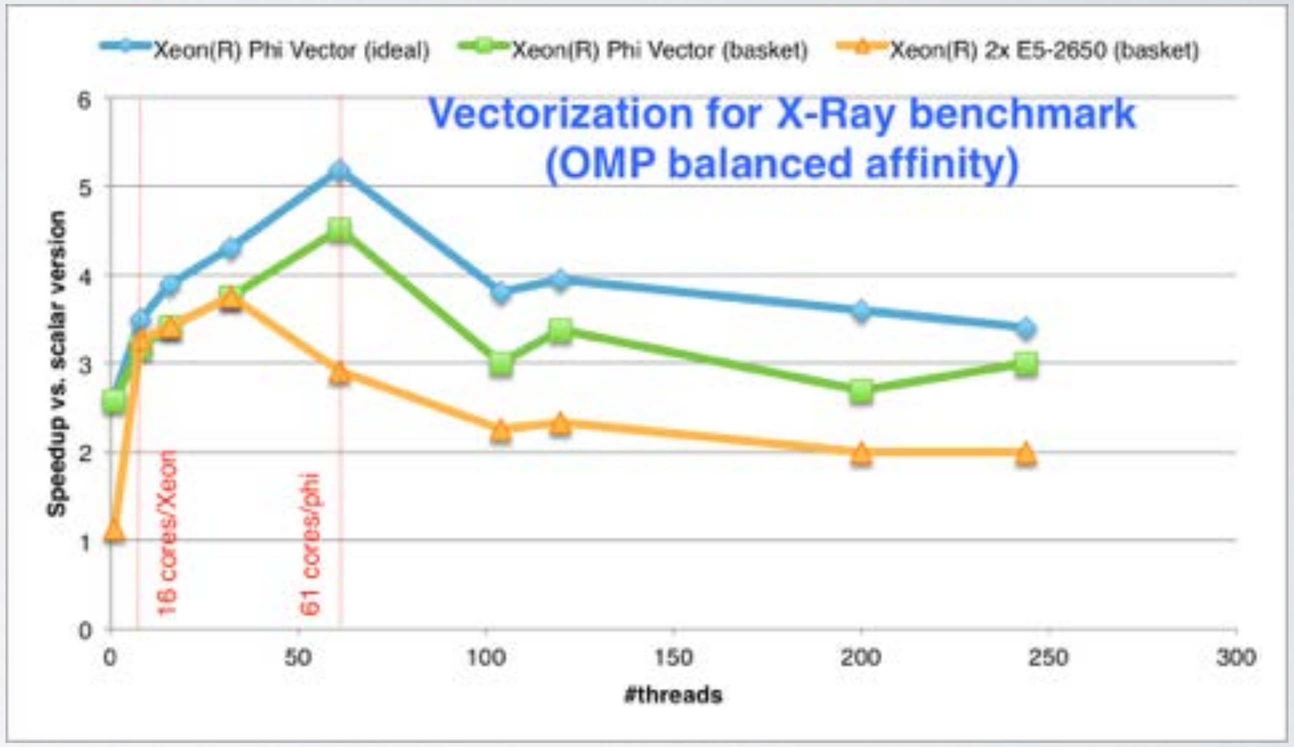
- Better behavior using OMP balanced
  - Approaching well the ideal curve up to native cores count
  - Balanced threading converges towards the compact model as all the thread slots are filled
- It's worth to run Xeon Phi saturated for our application
- The throughput performance for a saturated KNC is equivalent (for this setup) to the dual Xeon E5-2650L@1.8GHz server which hosts the card.





VECTOR PERFORMANCE

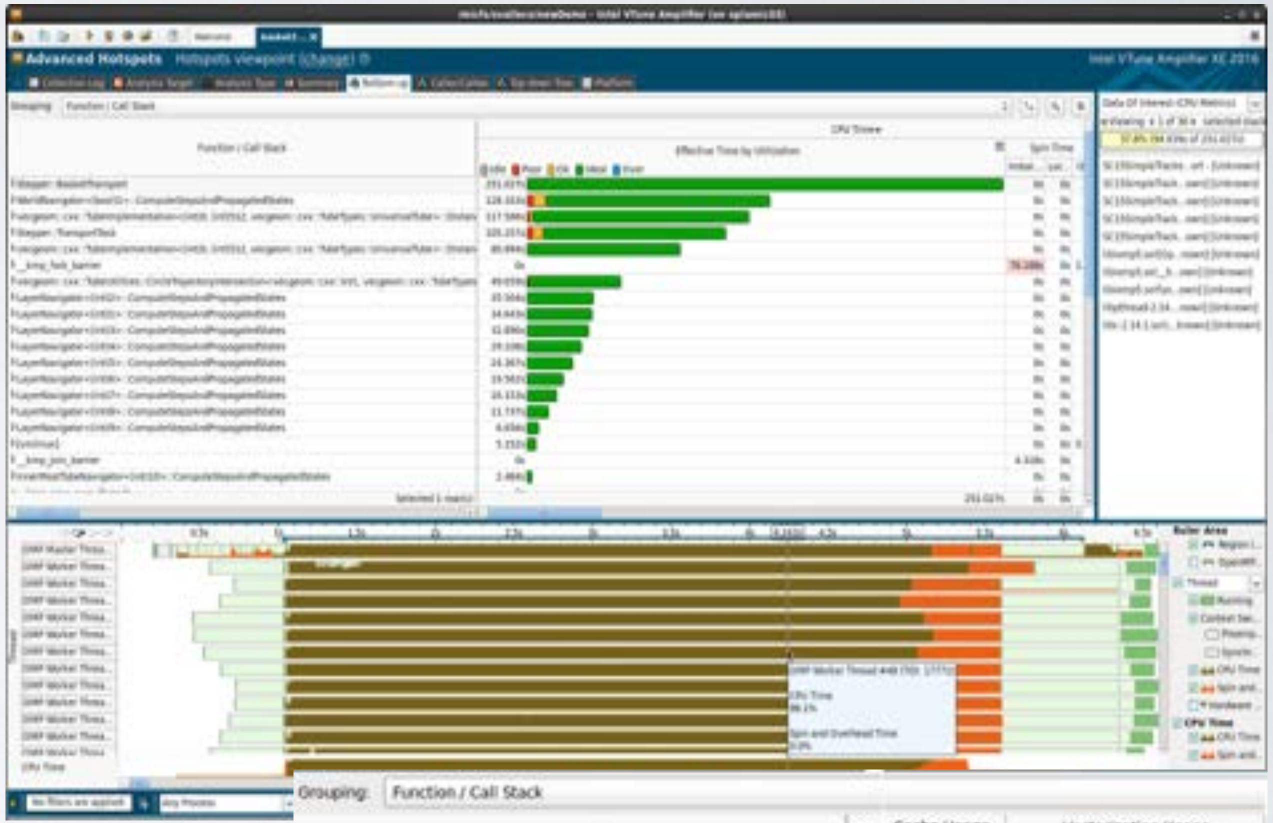
- Gaining up to 4.5 from vectorization in basketized mode
  - Approaching the ideal vectorization case (when no regrouping of vectors is done) .
- Vector starvation starts when filling more thread slots than the core count
  - Performance loss is not dramatic
  - Better vectorization compared to the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

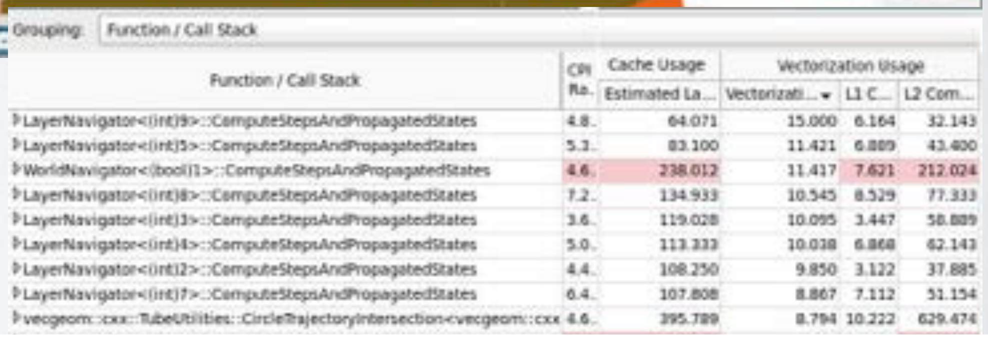


- Scalar case: Simple loop over pixels
- Ideal vectorization case: Fill vectors with N times the same X-ray
- Realistic (basket) case: Group baskets per geometry volume

PROFILING FOR THE X-RAY BENCHMARK

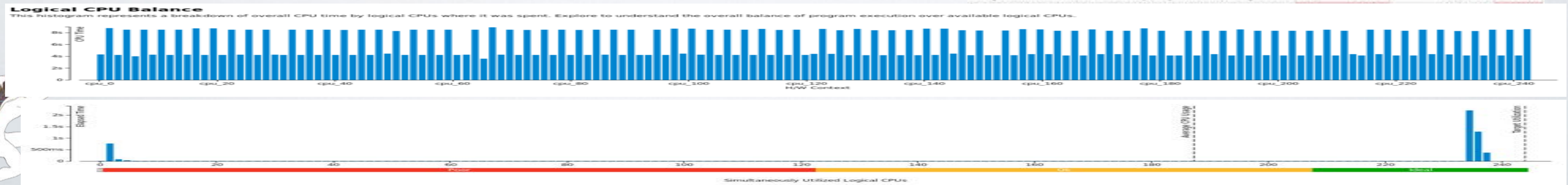
- Good vectorization intensity, thread activity and core usage for the X-Ray basketized benchmark on a Xeon Phi (61 core C0PRQ-7120 P)
- The performance tools gave us good insight on the current performance of GeantV





Grouping: Function / Call Stack

Function / Call Stack	CPI Ra..	Cache Usage	Vectorization Usage		
		Estimated La...	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



LOOKING FORWARD TO…

- … implementing a “smoking gun” demonstrator 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 and optimizing the workflow on KNL
  - Important architecture to test how flexible our model is
  - Expecting epic “fights” for scaling up the performance
- Complete the porting on GPUs and start performance optimization
- Already working on implementing device-specific scheduling policies and addressing NUMA awareness

SUMMARY

- We are designing the next generation simulation program architecture
    - SIMD exploitation and accelerators are the focus of this effort
- We have a prototype which looks promising toward our goal of a performance gain of a factor 3-5 over current software
- We plan to have a “testable” prototype in a couple of year from now (end 2017)
- We look forward to more communities joining our effort

PERSPECTIVES

- Doing HPC when you do not use blas-rich codes feels like being the “poor relation”
    - Benchmarks are of reduced relevance
    - Your CPI is poor / abysmal
    - There is little guidance on how to go ahead
- Moreover the “far-from-blas” community is sparse and communication is poor
    - HEP for one is seriously affected by NIH syndrome
- There is a nagging feeling of reinventing the (square) wheel
- Communication is here a major problem
    - Big data, ROOT…