Design, implementation and performance results of the GeantV prototype

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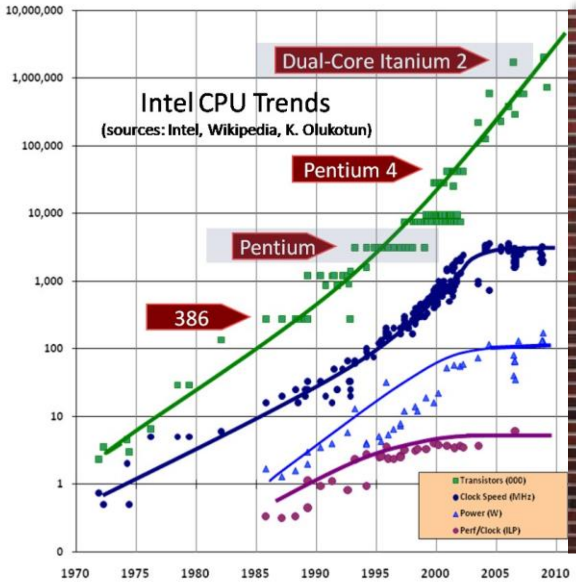
Draft v1

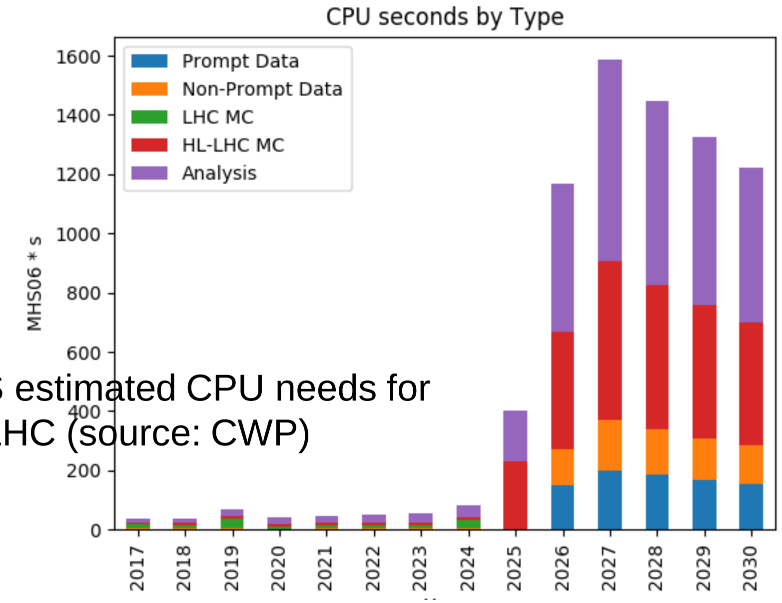
1. Introduction, context, motivation

Why?

Context

- Hardware requirements: hitting walls
  - power, ILP, memory access
  - -> multi/many cores with SIMD pipelines
- LHC requirements++: Run3->HL
  - Simulation still a bottleneck in many workflows
  - demand for simulated samples ~luminosity
- Application requirements: simulation is hard to optimize
  - Very complex stepping per track
  - Large code, sequential OO design from early C++ adoption era (deep stacks, virtual calls)
  - Small % silicon utilization





CMS estimated CPU needs for HL-LHC (source: CWP)

Application morphology: stepping

4. Propagate in field to reach selected step
Cross boundary

Charged particle in field

5. Post-propagation MSC step correction

2. Find next boundary + safety

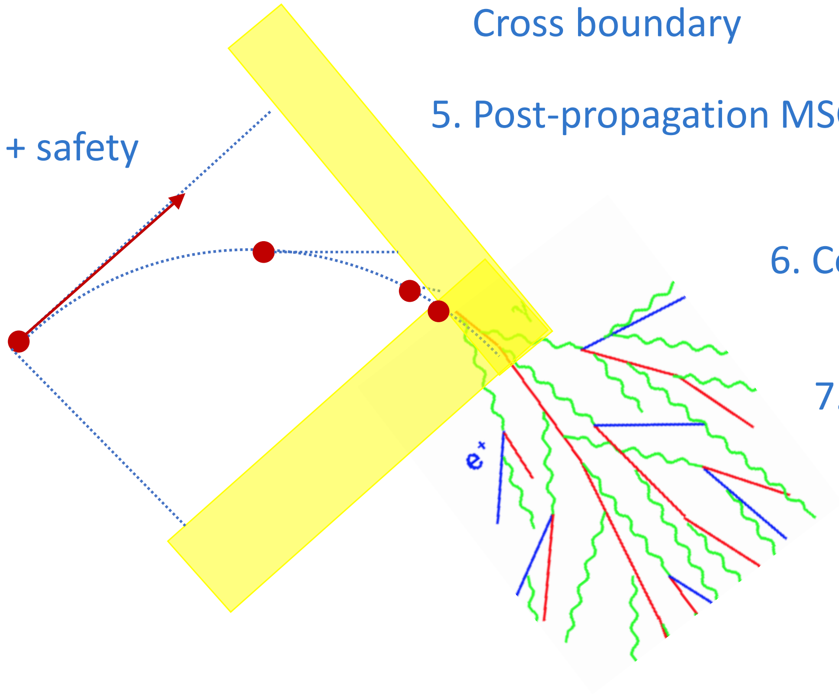
6. Continuous processes (ioni)

1. Sample interaction length:

7. Sample discrete process + at rest

3. Sample MSC

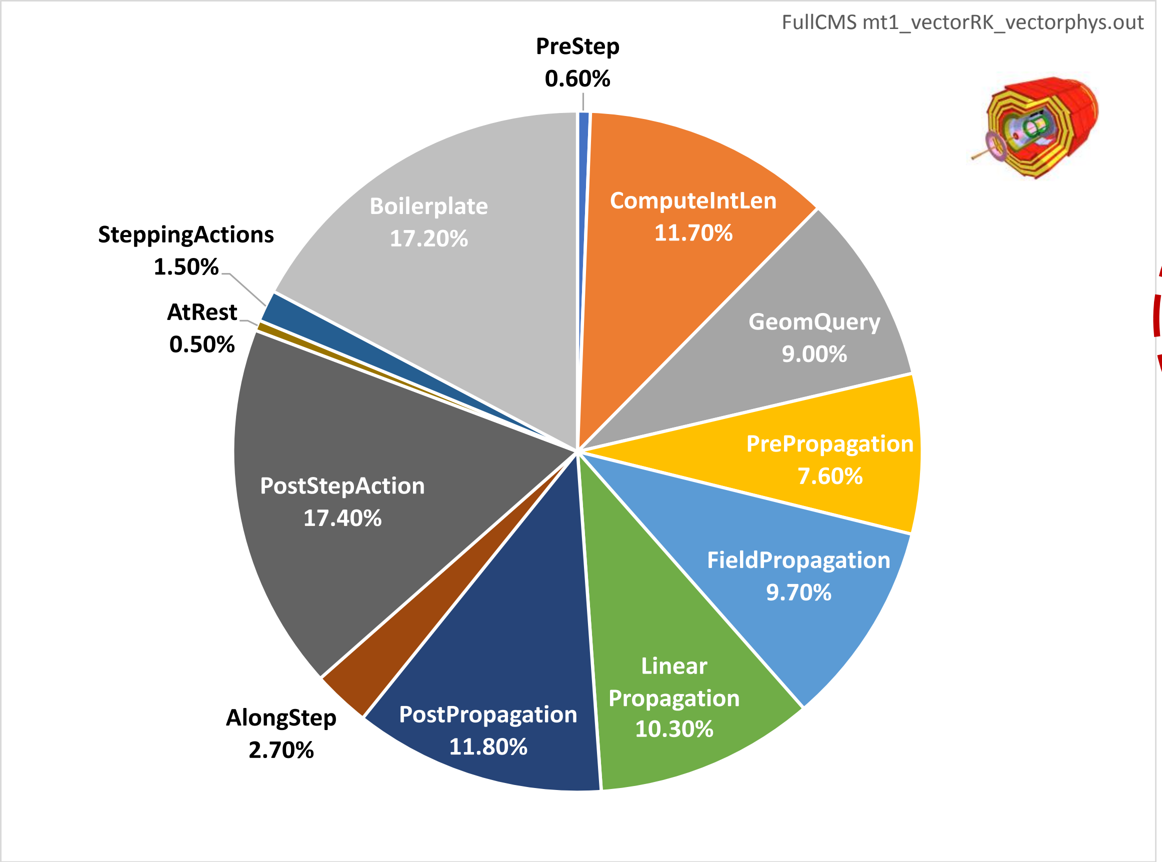
8. Stepping actions

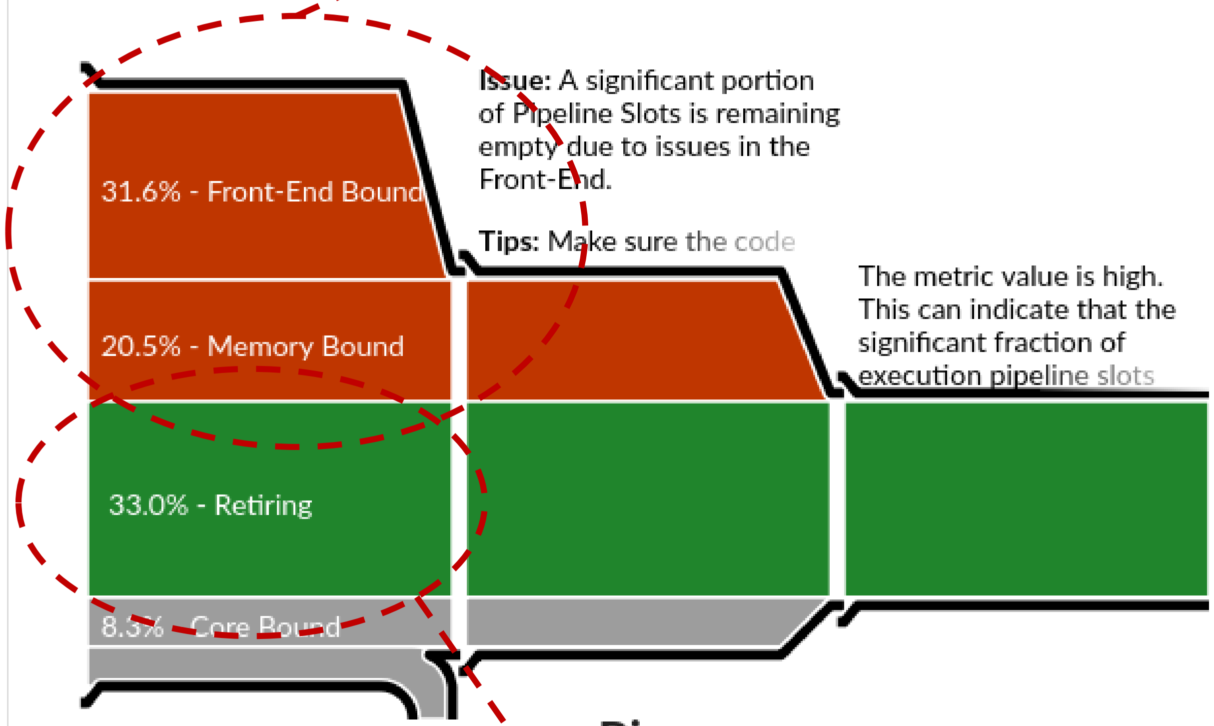


- The stages can make a pipeline, but each stage is large and complex (10^2-10^{4+} LOC, deep stacks, stochastic decision tree)
- Track state gets changed after every stage -> strong data binding between functional parts

Motivations: locality & vectorization

Get rid of those…





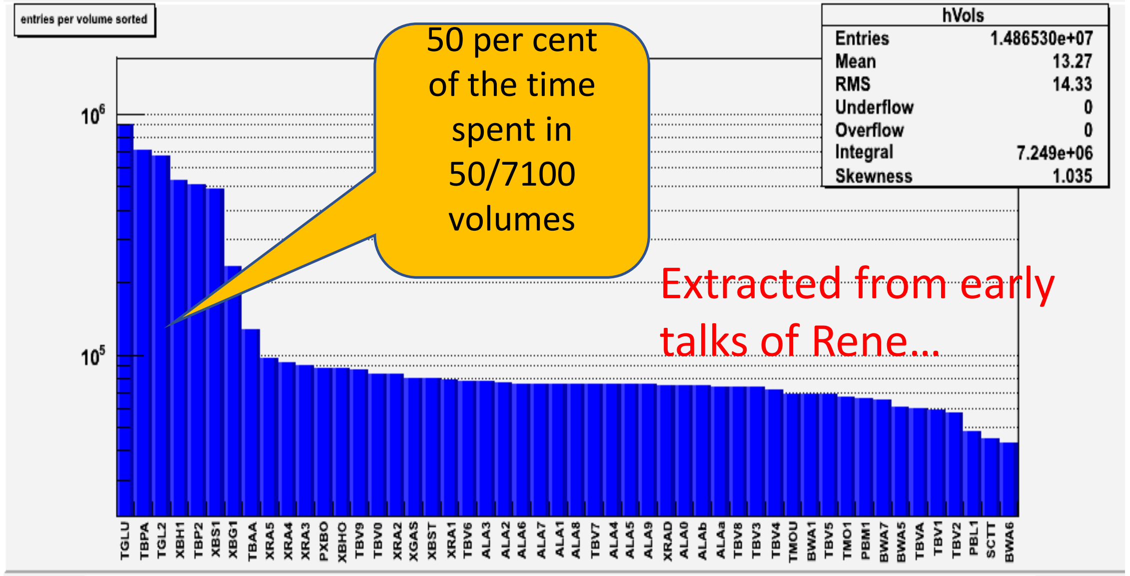
µPipe

The numbers are not absolute, they depend a lot on the application, they are however a guidance for what happens in a complex setup

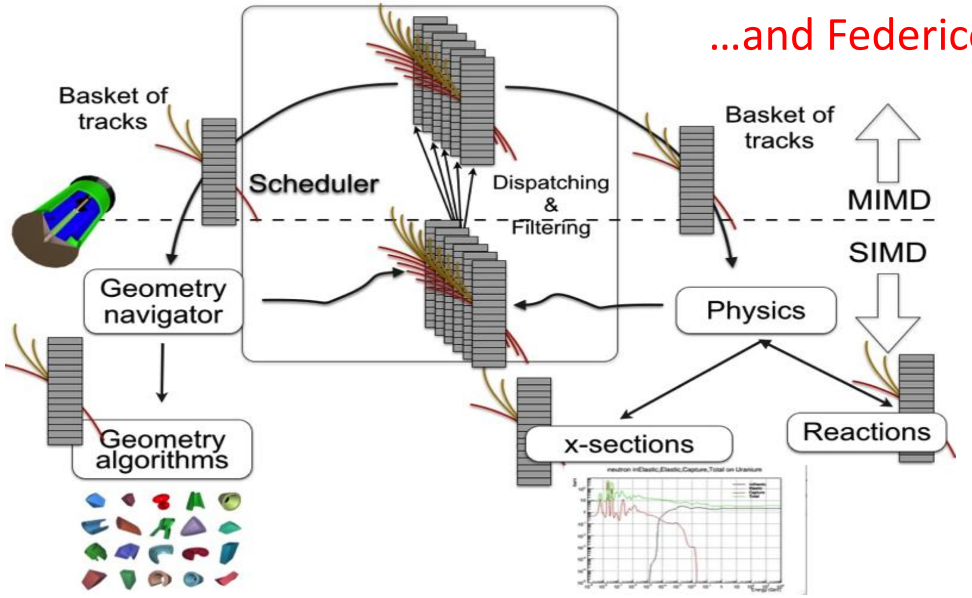
Shrink some cycles used here…

GeantV

- Initial observations
  - There is potential for locality in simulation
  - Locality opens up parallelism
- Initial ideas
  - Grouping tracks doing same work
  - make the work vectorizable on tracks
  - Gather tracks from more events to increase populations
- Initial goals
  - Factor 2-5 for **full sim**
    - increased locality and vectorization, usage of larger % of the hardware
  - New opportunities for accelerators
  - “Prototype with 2000 lines in few months” (2013) 😊



…and Federico



Initial challenge : vectorizing the outer loop?

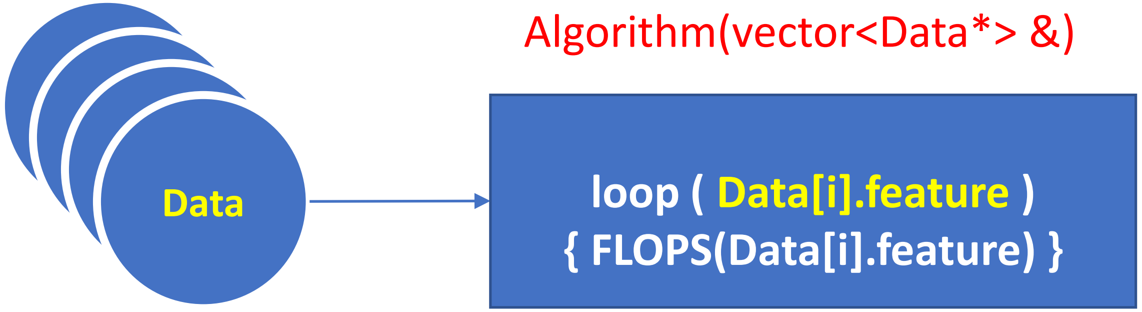
Model feature parallelism
(e.g. surfaces of a polyhedron)

Algorithm(Data &, ModelState& m)

Not so many algorithms with natural inner loops

Data feature parallelism
(e.g. multiple tracks)

Algorithm(vector<Data*> &)



Needs track-parallel environment

Modifying the workflow involves more copy overhead, since m.feature may be const data vector while data[i].feature needs to be gathered -> vector FLOPS need to worth it

2. Concepts, design considerations

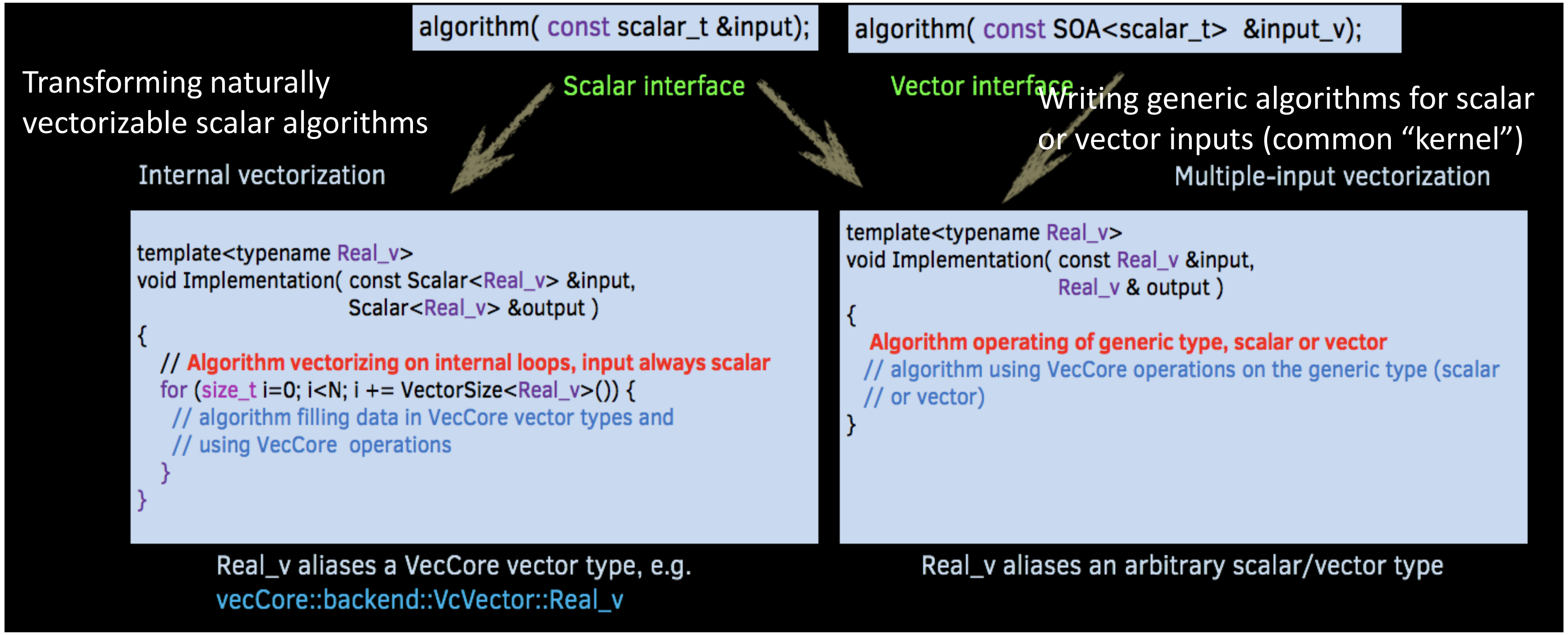
Can it be done?

Data processing oriented design

- Bundle work of the same type -> make it look more like pipeline
  - Need more tracks doing the same work -> “basket”
  - Tracks will need to be regrouped -> state fully contained in track
    - Reentrant methods with tracks/baskets as arguments -> API change
- Enable data locality
  - Tracks in baskets need to be nearby in physical memory -> basket = SOA
- May need to reinforce basket populations
  - Allow several events in flight -> event slots
- … concurrently
  - Shared basket data structure with atomic synchronization -> extra complexity

Code redesign: vector interfaces

- Reusing code -> templated kernels for scalar/vector data types
- Geometry locality and basket-aware navigation -> VecGeom
- Enforcing short vectorization -> support different vectorization types

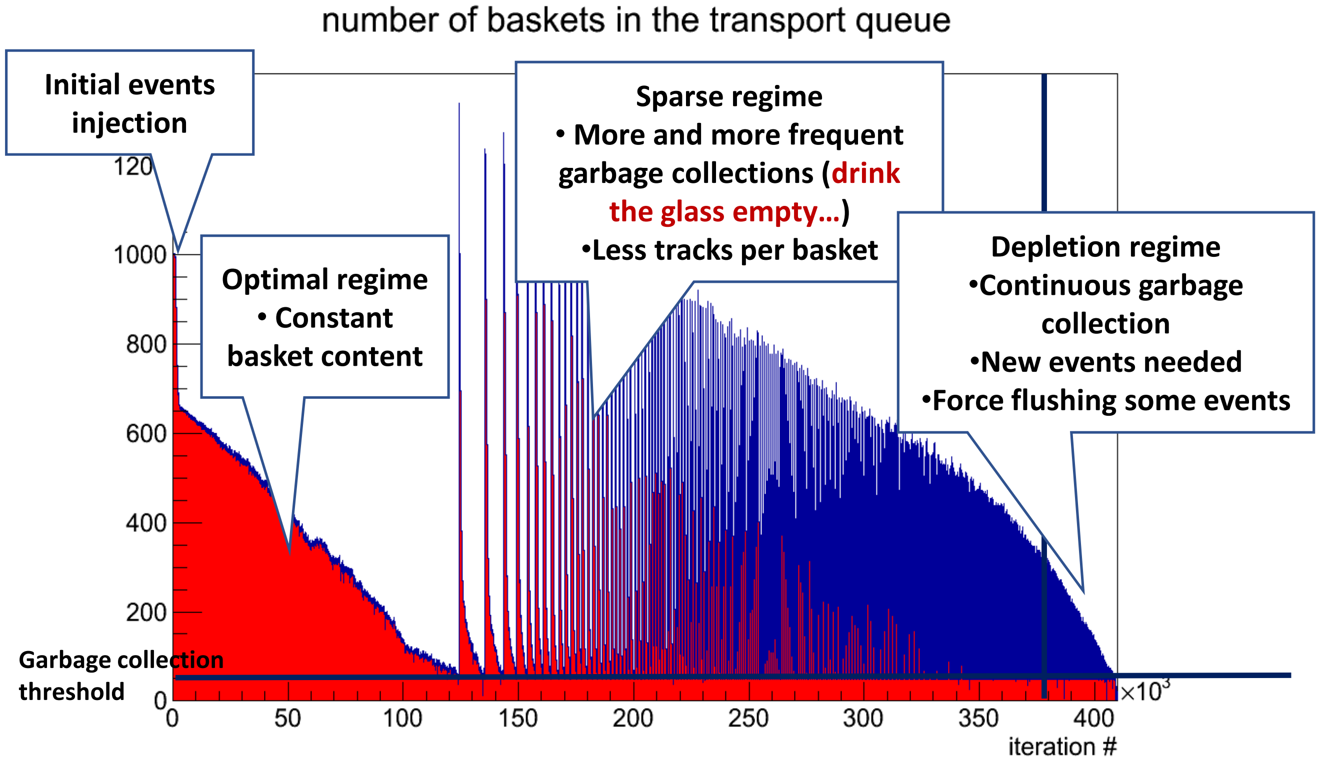


Prototyping revealed unforeseen problems

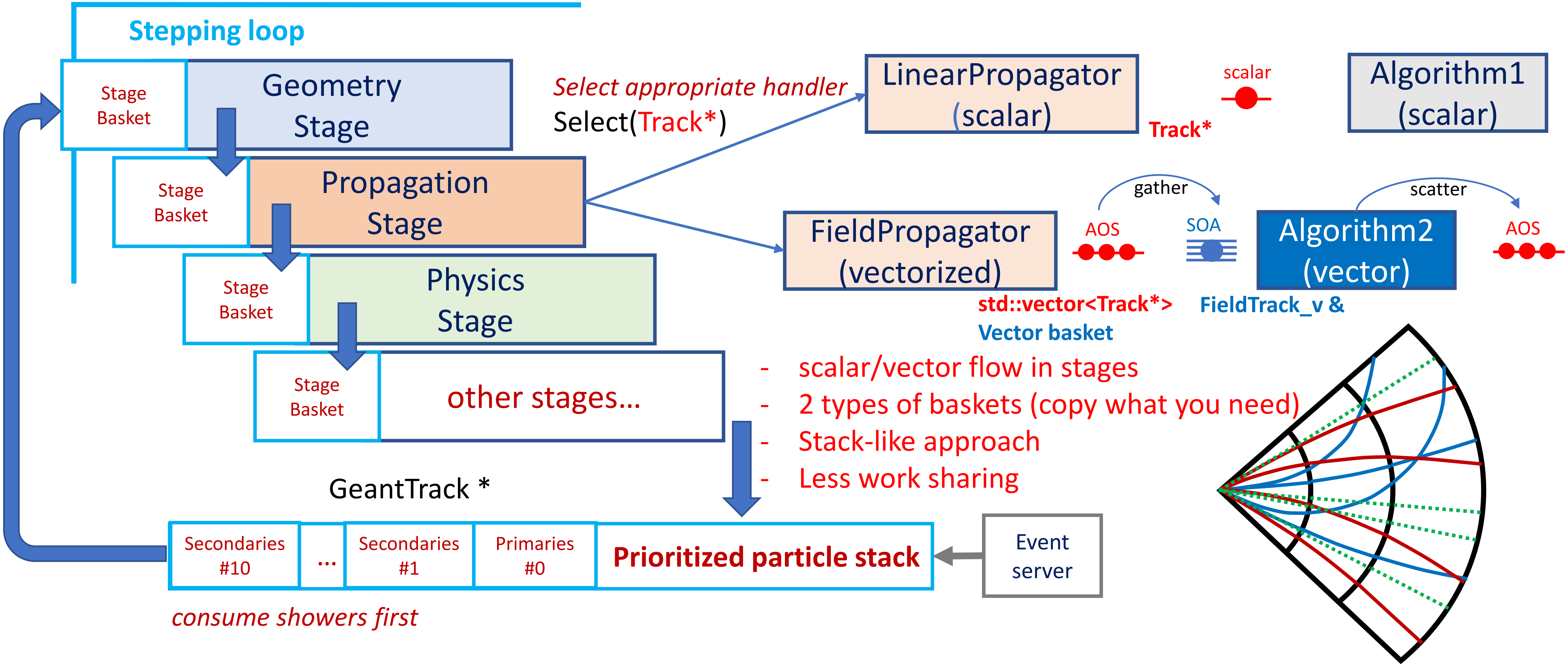
- Track populations executing different kernels are not uniform
  - Putting one basket per logical volume requires lots of tracks to trigger basket processing on a threshold
- Gathering many tracks implies also inefficient flushing
  - Otherwise bundling too much work prevents events from finishing
- Concurrent track gathering in general track SOA creates bottlenecks
  - Scaling problems, but also useless data copying
- Boosting both instructions and data locality in simulation has a price
  - Copy the state…

About 2000 lines, one year later…

- A lot of good signs and hopes
    - Geometry components showing good vectorization
- Revealed how complex the problem really was…
    - …and how reality can be different from blackboard drawings
- Dealing with extra complexity and seeking solutions since then
    - Moving gradually from a toy example with geometry only to the full complexity of an LHC experiment simulation



Going complex: algorithm-oriented design



Concurrency design

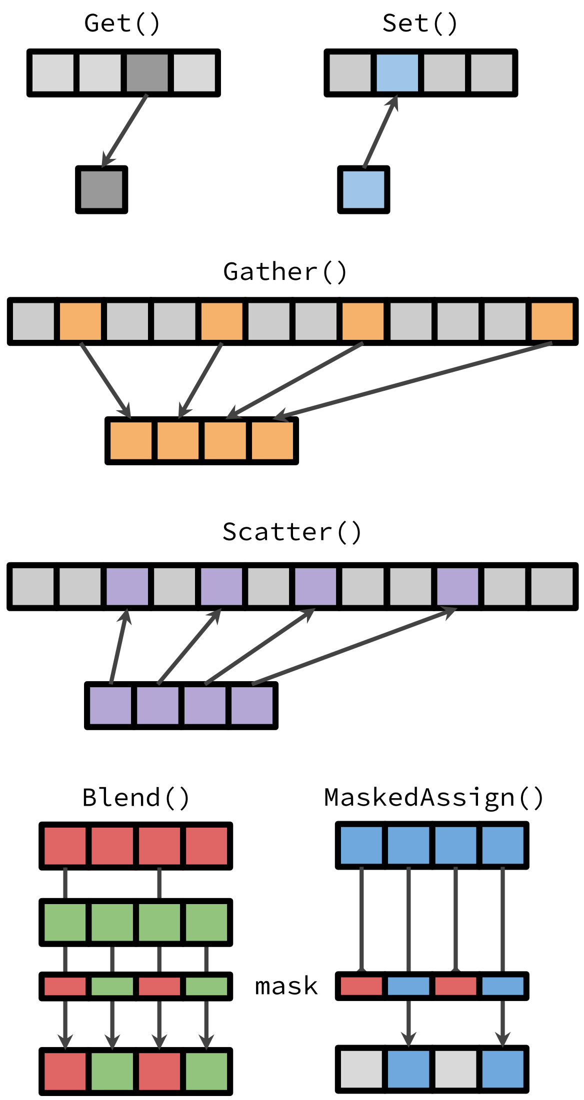
- Minimize context switches: single kernel thread model (worker) vs. TBB-base attempts
- Event slots: thought as a necessity…
  - More data for same work
- Track versus event level parallelism: try to find the optimum
  - Be able to share state data, but exchange the minimum
- Support for externally-driven parallelism
  - What are HEP concurrent frameworks happy with?
- Towards functional programming style: percolating all state (task data & tracks) through interfaces, making functions fully re-entrant

3. Implementation: the components

How?

VecCore – SIMD Abstraction Library

- Simple API abstracting common SIMD operations in a generic way
- Evolution of “backends” from VecGeom
- Became a standalone library in 2017: https://github.com/root-project/veccore
- Used by VecGeom and ROOT
- Supports SIMD in x86_64 via Vc and UME::SIMD, SSE2 to AVX512
- Supports ARM, PPC64 with scalar backend
- Supports Windows, Mac, and Linux



VecGeom – vectorized geometry library

- Workhorse for implementing the main project ideas:
  - Multi-architecture support, scalar/vector workflows
  - Multi-level vectorization (optimization structures + shape algorithms)
- Performance-driven development
  - best algorithms inspired from GeantV/ROOT/USolids
- Production-level quality
- Unit-tests showing excellent performance figures
- Main problem: dispatching efficiently to lower level algorithms
  - Cannot group by boxes/tubes/…, but only by logical volumes
  - Volume navigation has to talk to several daughters -> work divergence

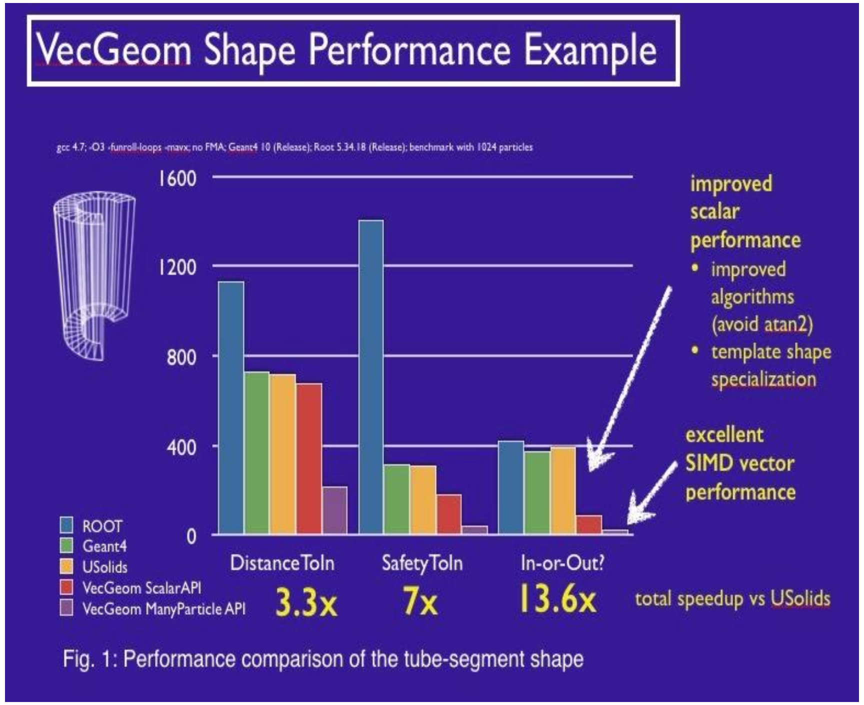
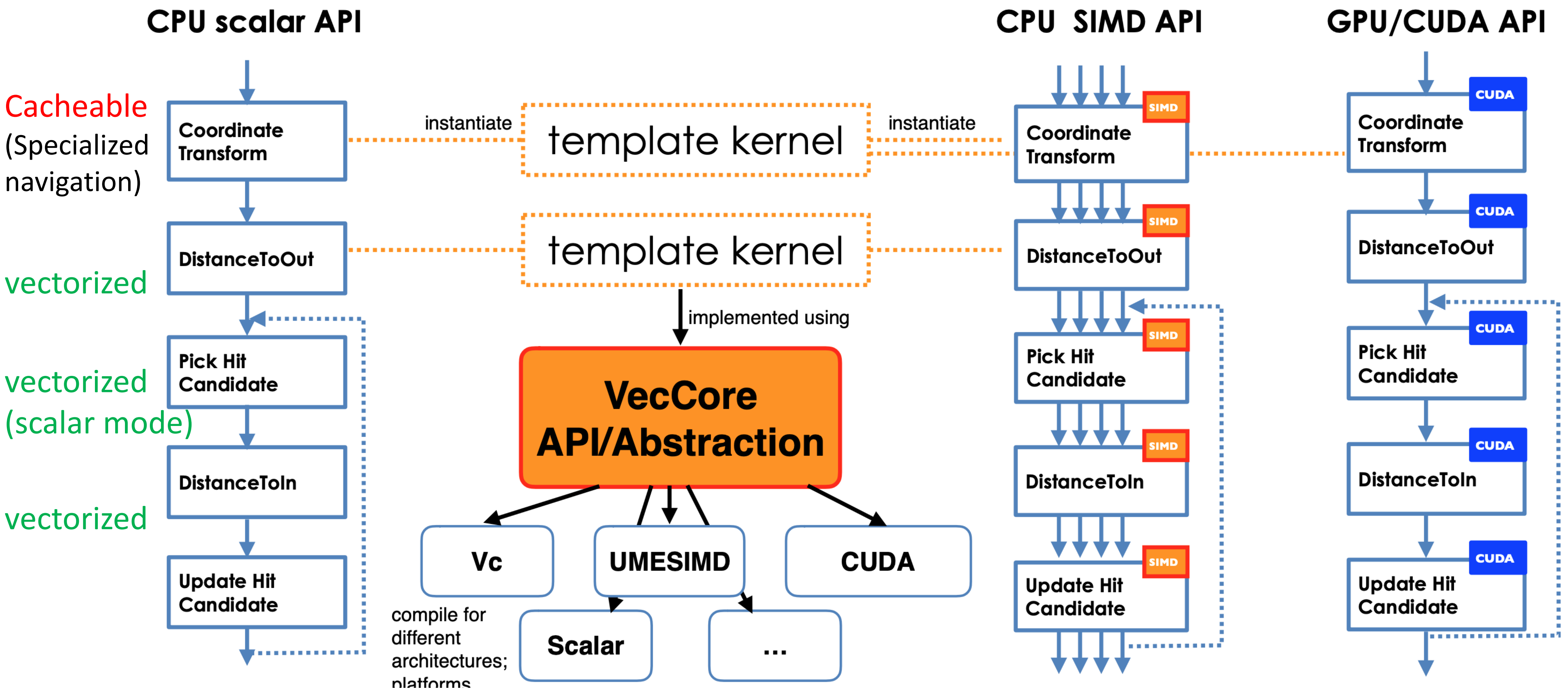


Fig. 1: Performance comparison of the tube-segment shape

VecGeom code organization

gitlab.cern.ch/VecGeom/VecGeom



VecMath: vectorization support for math utilities

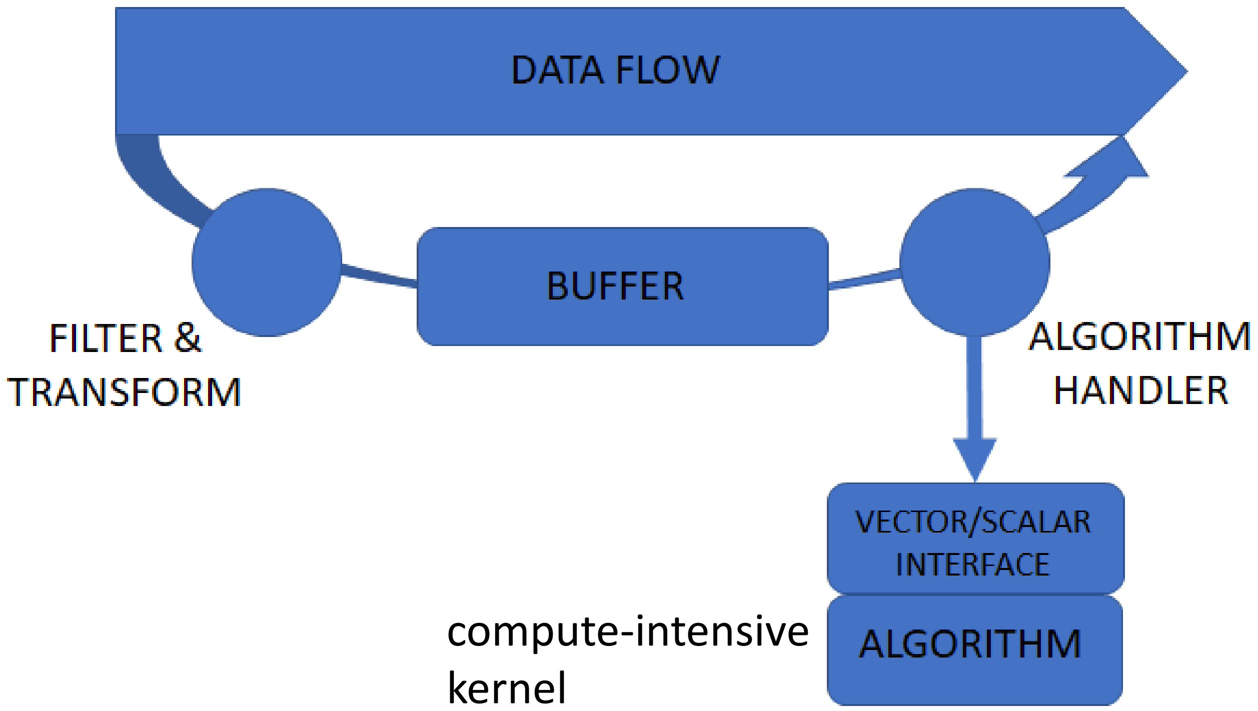
github.com/root-project/vecmath

- Library needed for common vectorized algorithms, math, vector-aware types (Vector3D, SOA3D, AOS3D, …)
  - For now only: PRNG implementations, fast math functions (vectorized)
- Idea: extending the library to provide common vectorization support
  - Migrate existing common stuff from VecGeom & GeantV, add extra general-interest utilities

VectorFlow: generic vector adapter scalar workflows

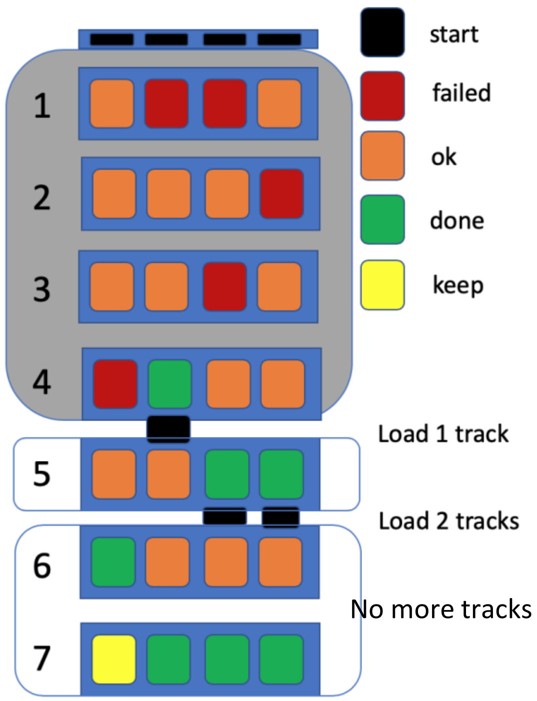
- A way to express outer loop vectorization in a general way in a *scalar workflow*
- Templated abstraction based on the concepts of *'work'* and *'flow'* inspired by GeantV
- Extracted as independent library
- Using VecCore as underlying vectorization library

https://github.com/agheata/vectorflow



Integration of motion in Field

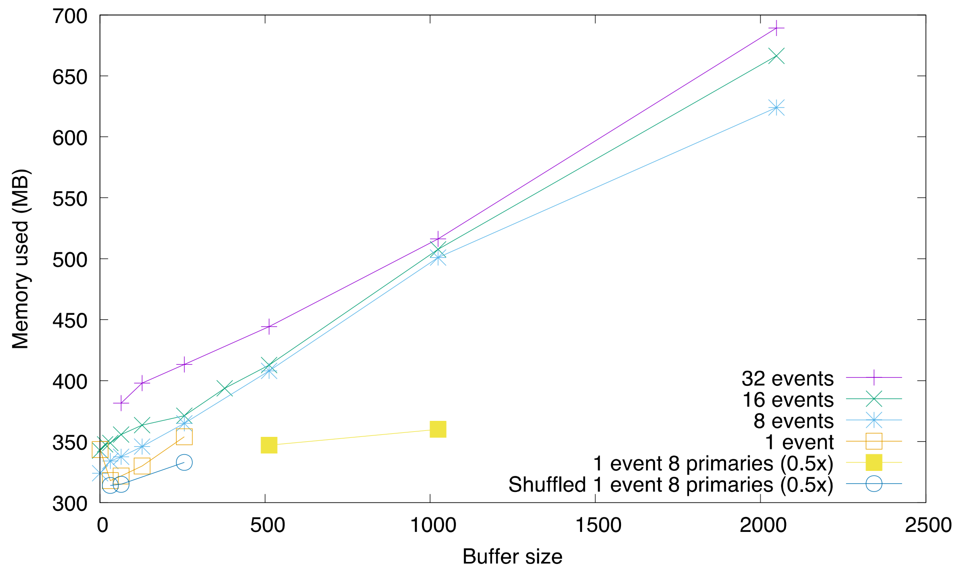
- Integration takes about 18% CPU time in 'scalar' GeantV
- Lower level classes 'simply' vectorizable
  - Implementation templated on Field/Equation types
- Top level 'Driver' fully rewritten
  - checks good step and end of integration, reloads lanes with new work.
- Separate basket size 'b' configured for field propagation
  - Lanes doing useful work increases with 'b'
  - Memory size increases – by 160MB for b=1024



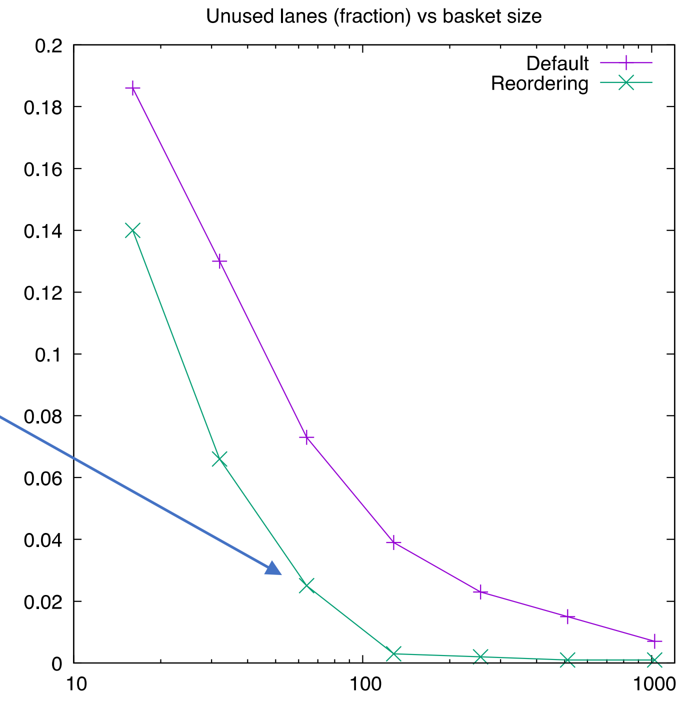
Field Propagation - results

- Efficiency and memory use depend strongly on basket size b
  - Lanes doing useful work increases from 82% (b=16) to 99.3% (b=1024)
  - Memory size increases – by 160MB for b=1024 (16 event window) (why?)
- Further refinements possible
  - ‘Reordering’ tracks - so long integration moves to basket front (tested – 97.5% util. @ bsz=64)
  - Using ‘single’ track code if only 1 track is left.
  - Improved load / store.

Move to results section?



Memory size vs ‘field’ basket size for different event window sizes.



GeantV EM physics models

particle	processes	models(s)	
		GeantV	Geant4 defaults
e^-	ionisation	Møller[100eV-100TeV]	Møller[100eV-100TeV]
	bremsstrahlung	Seltzer-Berger [1keV-1GeV]	Seltzer-Berger [1keV-1GeV]
		Tsai (Bethe-Heitler) w. LPM. [1GeV-100TeV]	Tsai (Bethe-Heitler) w. LPM. [1GeV-100TeV]
	Coulomb sc.	GS MSC model [100eV-100TeV]	Urban MSC model [100eV-100TeV]
			Mixed model [100MeV-100TeV]
e^+	ionisation	Bhabha [100eV-100TeV]	Bhabha [100eV-100TeV]
	bremsstrahlung	Seltzer-Berger [1keV-1GeV]	Seltzer-Berger [1keV-1GeV]
		Tsai (Bethe-Heitler) w. LPM. [1GeV-100TeV]	Tsai (Bethe-Heitler) w. LPM. [1GeV-100TeV]
	Coulomb sc.	GS MSC model [100eV-100TeV]	Urban MSC model [100eV-100TeV]
			Mixed model [100MeV-100TeV]
	annihilation	-Heitler (2γ) [0-100TeV]	Heitler (2γ) [0-100TeV]
γ	photoelectric	Sauter-Gavrila + EPICS2014 [1eV-100TeV]	Sauter-Gavrila + EPICS2014 [1eV-100TeV]
	incoherent sc.	Klein-Nishina$^+$ [100eV-100TeV]	Klein-Nishina$^+$ [100eV-100TeV]
	e^+e^- pair production	Bethe-Heitler$^+$ [100eV-100TeV]	Bethe-Heitler$^+$ [100eV-100TeV]
		Bethe-Heitler$^+$ w. LPM [80GeV-100TeV]	Bethe-Heitler$^+$ w. LPM [80GeV-100TeV]
	coherent sc	-	Livermore
+	energy loss fluct.	-	Urban

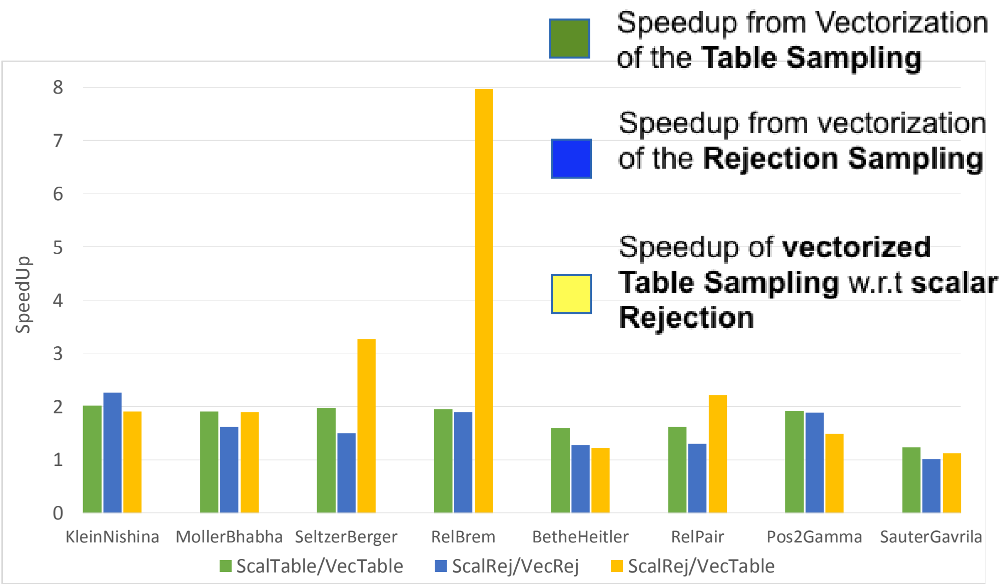
GeantV physics list used also in Geant4 for comparisons

Vectorized EM physics models

- Revised models describing ~complete EM physics (except energy loss fluctuations)
  - More compact implementations, simplified interfaces
  - Support for multiple physics list
  - Several features went back also in Geant4, so the physics Geant4/GeantV can be numerically compatible
- All the models are multi-particle vectorized
  - Most important work was done to vectorize the common services: sampling algorithms (alias, table), track rotation/boost
  - Many challenges: unpredictable recursions, memory access, code complexity
  - **Final state EM speedup**: between **1.5-3** on Haswell, **2-4** on Skylake with **AVX2**
- Most efficient implementation for a model depends on many factors
  - Energy, material composition
  - The full performance study is not complete

Main lessons from physics vectorization

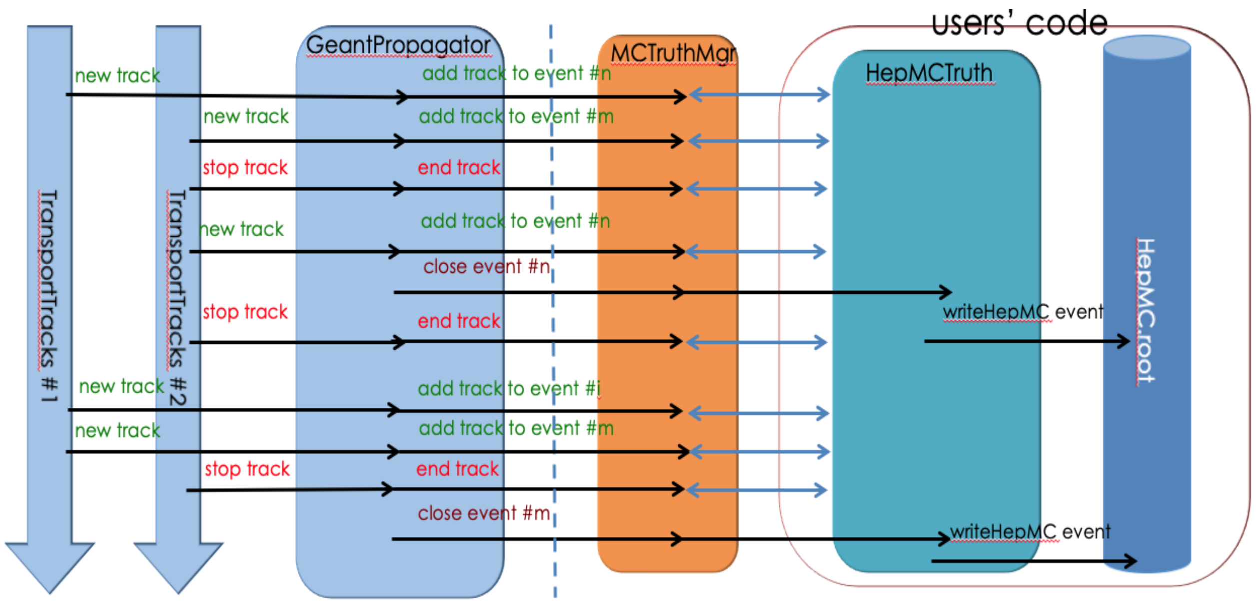
- There is **no generic solution** to achieve speedup
  - The best approach is often a compromise
    - E.g. choosing sampling method to be used
- Complex code can be also vectorized, but it has to worth the hotspot
  - There are “important” and ”less important” models depending on the simulation, ranging from < 1% to 4-5% of the total time
- Compactness and more efficient data access brings eventually much more benefits than vectorization for “small” hotspots



M. Bandieramonte, M. Novak

MC truth: keeping track of kinematics

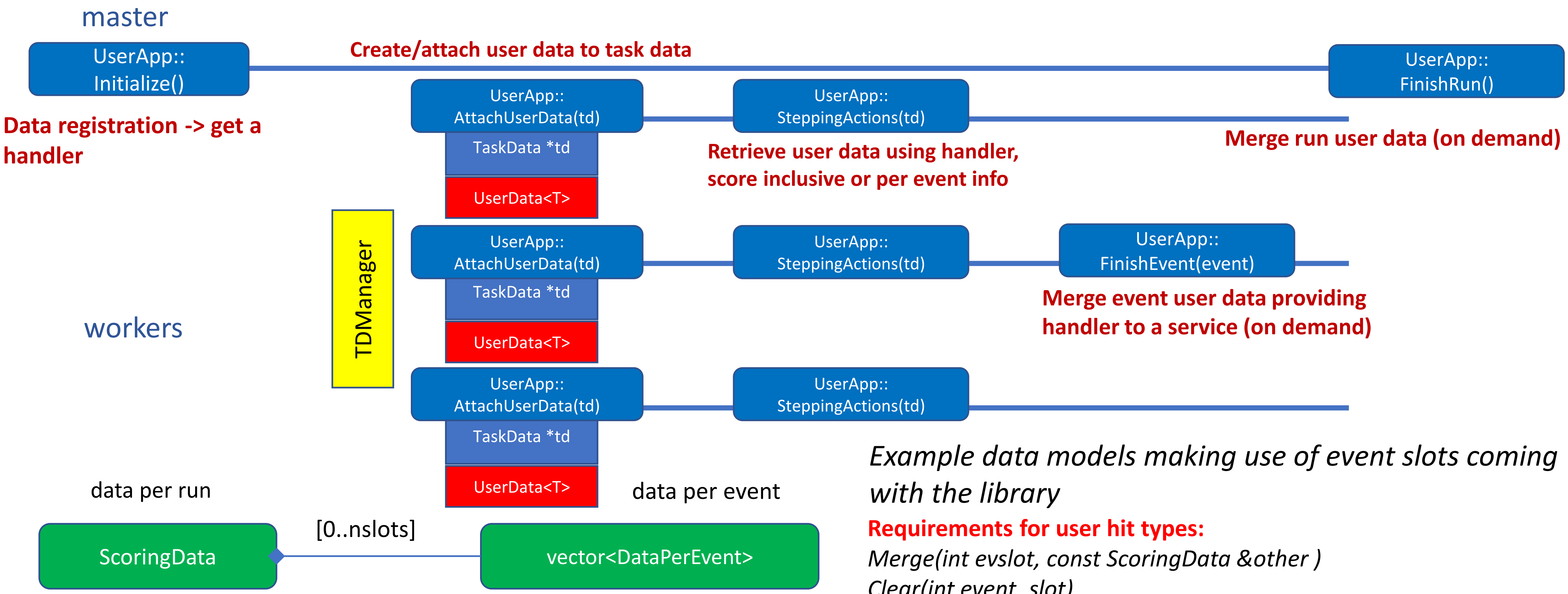
- we need to store the particle history necessary to understand the given event (process)
  - there is no single solution that would cover all use cases
  - functionality is provided as a user-hook allowing concrete user implementations
- interface (MCTruthMgr) implemented in the prototype
  - receives (concurrent) notifications from transport threads about: adding/ending particles, events finishing
  - delegates processing of particles history to concrete MC truth implementation
- Light coupling to transport
  - minimal 'disturbance' to transport threads
  - maximal flexibility of implementing custom particle history handlers
- concrete example implementation provided based on HepMC3
  - See backup slides for more details



User interfaces: a compromise

- Same callbacks as in Geant4, but dealing with the extra complexity of multiple events and multiple threads
  - Data structures: templated approach (users provide their own types)
  - Data indexed only by event slot, not thread id
- Approach changed from:
  - *“give me your hit model, I give you factories and tools to handle and store them efficiently concurrently”*
    - Nice concurrent merging service ending up in ROOT (TBufferMerger)
- To:
  - *“Here are the hooks allowing to allocate your own data and providing per-thread handles”*
  - *“Here is the workflow allowing to score concurrently and merge hit information”*
- Storing the hits or passing them to digitization is the user business

User data integration in GeantV callbacks



Example data models making use of event slots coming with the library

Requirements for user hit types:

Merge(int evslot, const ScoringData &other)

Clear(int event_slot)

4. Integration with experiment frameworks

Easy to use?

GeantV Integration in CMSSW

- Integration testing of GeantV w/ CMSSW has several goals:
  - Demonstrate benefits of co-development between R&D team & experiments
  - Exercise capabilities of CMSSW framework to interface with external processing (ExternalWork mechanism) and handle track-level parallelization in detector simulation
  - Measure any potential CPU penalties or gains when running GeantV in CMSSW
  - Estimate cost of adapting to new interfaces and eventually migrating to new (and potentially backward-incompatible) tools such as GeantV
    - Thinking forward to HPC/GPU solutions
- *Not* planning to migrate CMS simulation to GeantV
  - This is an R&D exercise

Overview of the integration exercise

- Exercise and debug features of GeantV and CMSSW
  - Run GeantV using CMSSW ExternalWork feature:
    - Asynchronous, non-blocking, task-based processing
  - Resolved impedance mismatch between original GV scheduler and CMSSW
- Template wrappers for Sensitive detectors (SD) and scoring
  - Ensure exact same SD code used for Geant4 & GeantV
  - Minimize overhead (no branching or virtual table)
  - Handle that each event processed in multiple threads, mixed in with other events (i.e. merge at end of each event processing)
- Performance results and conclusions discussed in separate sections

Conclusions from CMSSW integration

- CMS studies met ~all goals laid out
  - Co-development led to improvements and bug fixes in GeantV to facilitate experiments' use
  - One of the first projects to exercise CMSSW ExternalWork feature
  - Physics validation & CPU measurements show very positive results
  - Path to adapt interfaces efficiently is laid out
- Demonstrator to test major elements of GeantV-CMSSW integration is ready
  - Up to 2.6× speedup in CMSSW application
  - More efficient use of CPU caches in GV seems to translate in improved performance within CMSSW
  - The CMS simulation group thanks the GeantV R&D team for providing support to this integration exercise and making it a successful co-development endeavor.

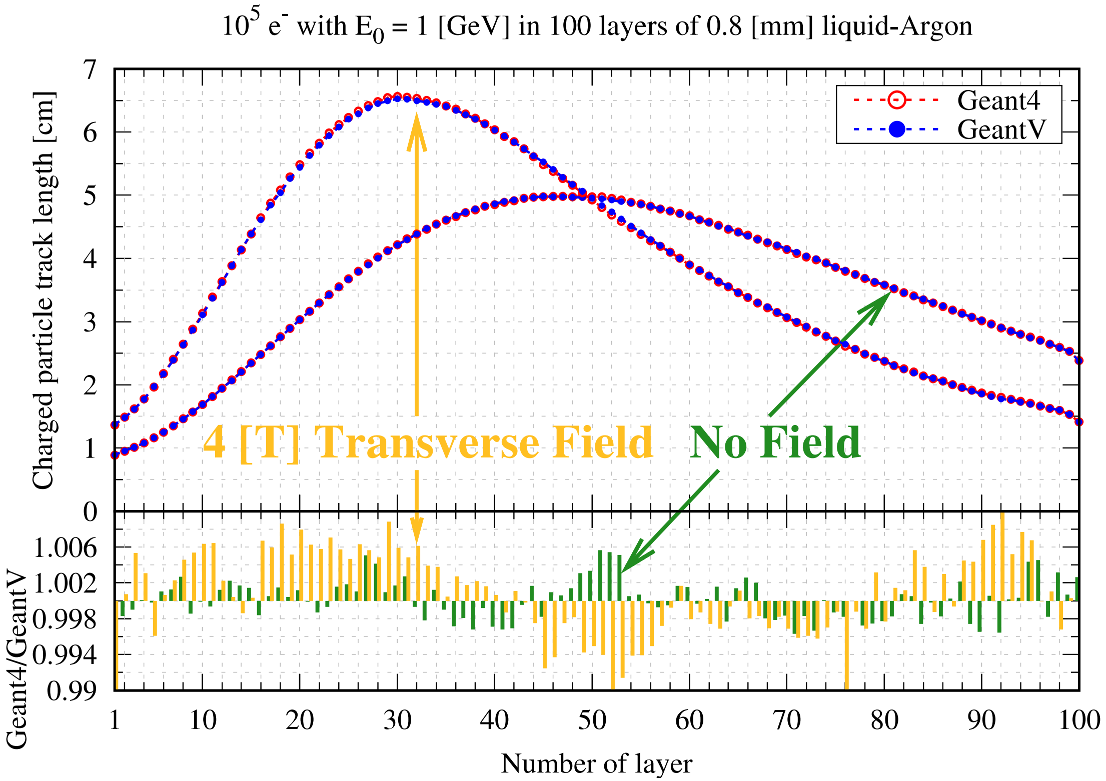
5. Performance results

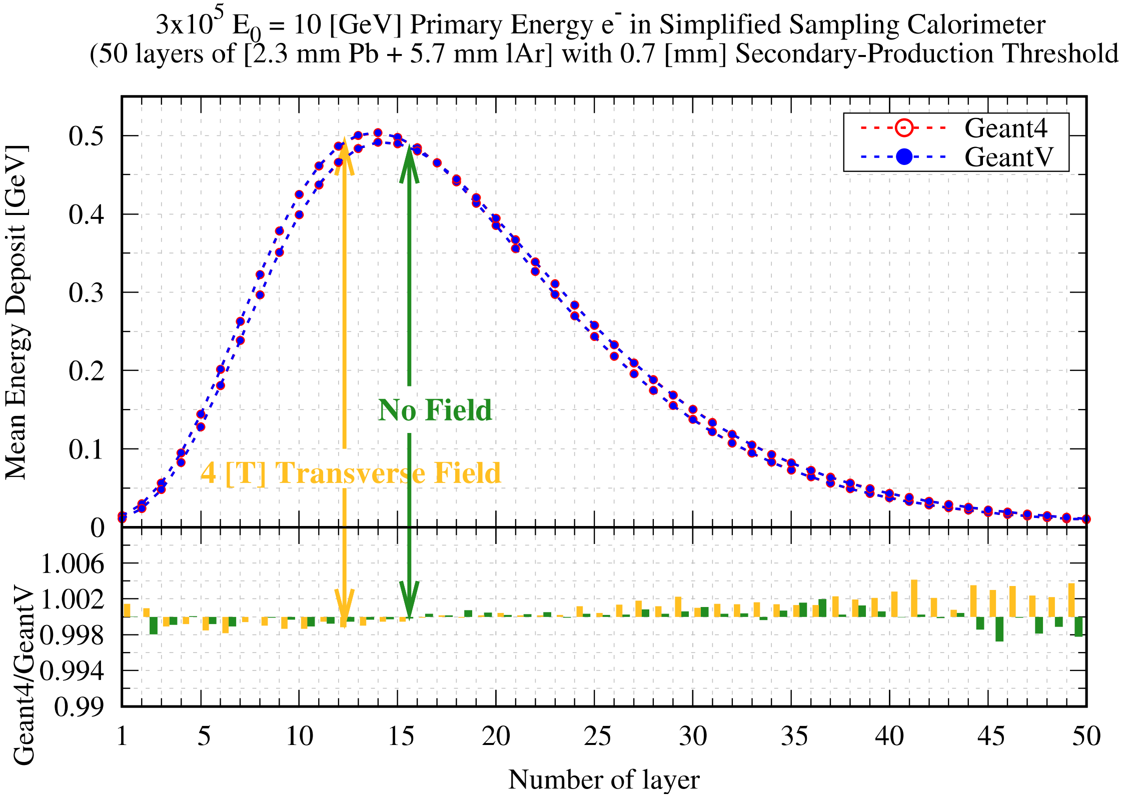
Is it efficient?

Benchmarks

- Set of application examples to demonstrate functionality and/or measure performance
  - Simple setups: thin layer, semi-infinite block, simplified sampling calorimeter
  - Complex setups with general non-experiment specific stepping actions: CMS, LHCb, extendible to other experiments
    - Full geometry and production cuts
    - Shooting electrons to fire EM physics
    - Allowing to tune internal GeantV parameters
    - GeantV and Geant4 applications mapped 1 to 1 (geometry, physics lists, gun, cuts)
- Set of CPU platforms, but also GPU
  - Different architectures, CPU, cache configurations
  - Performance results given mostly for the CMS benchmark

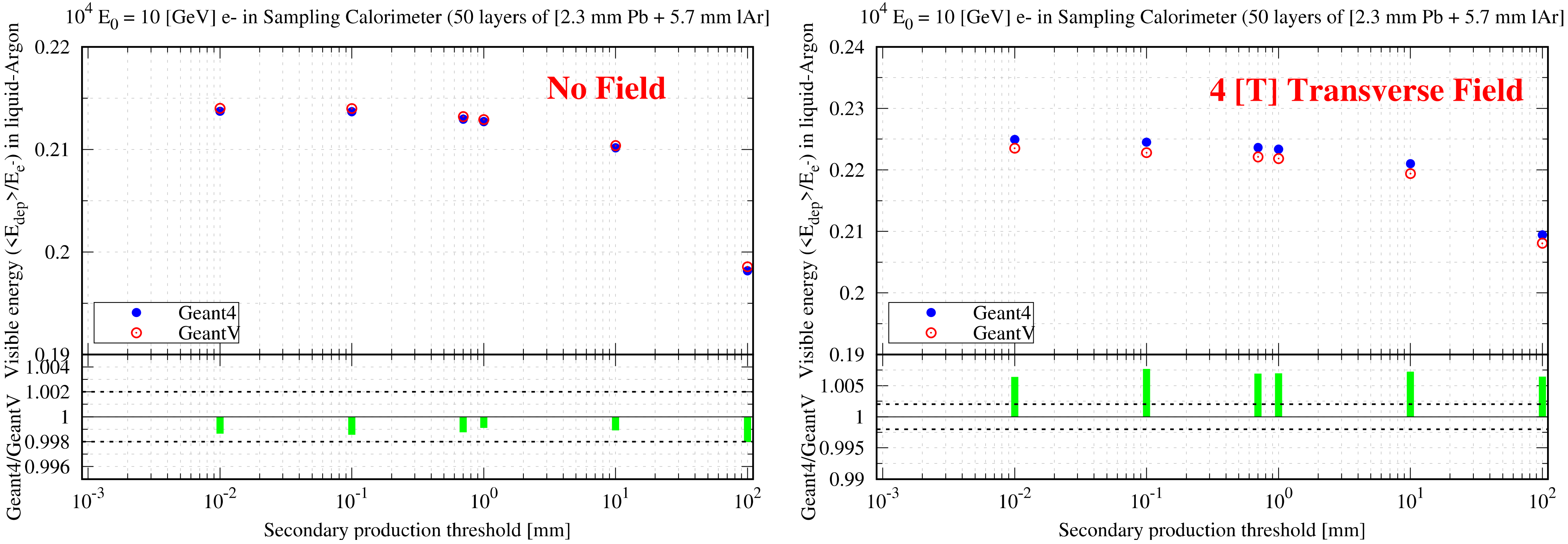
Getting same results for same simulation (1)





- Per-mil agreement for all observables in most cases

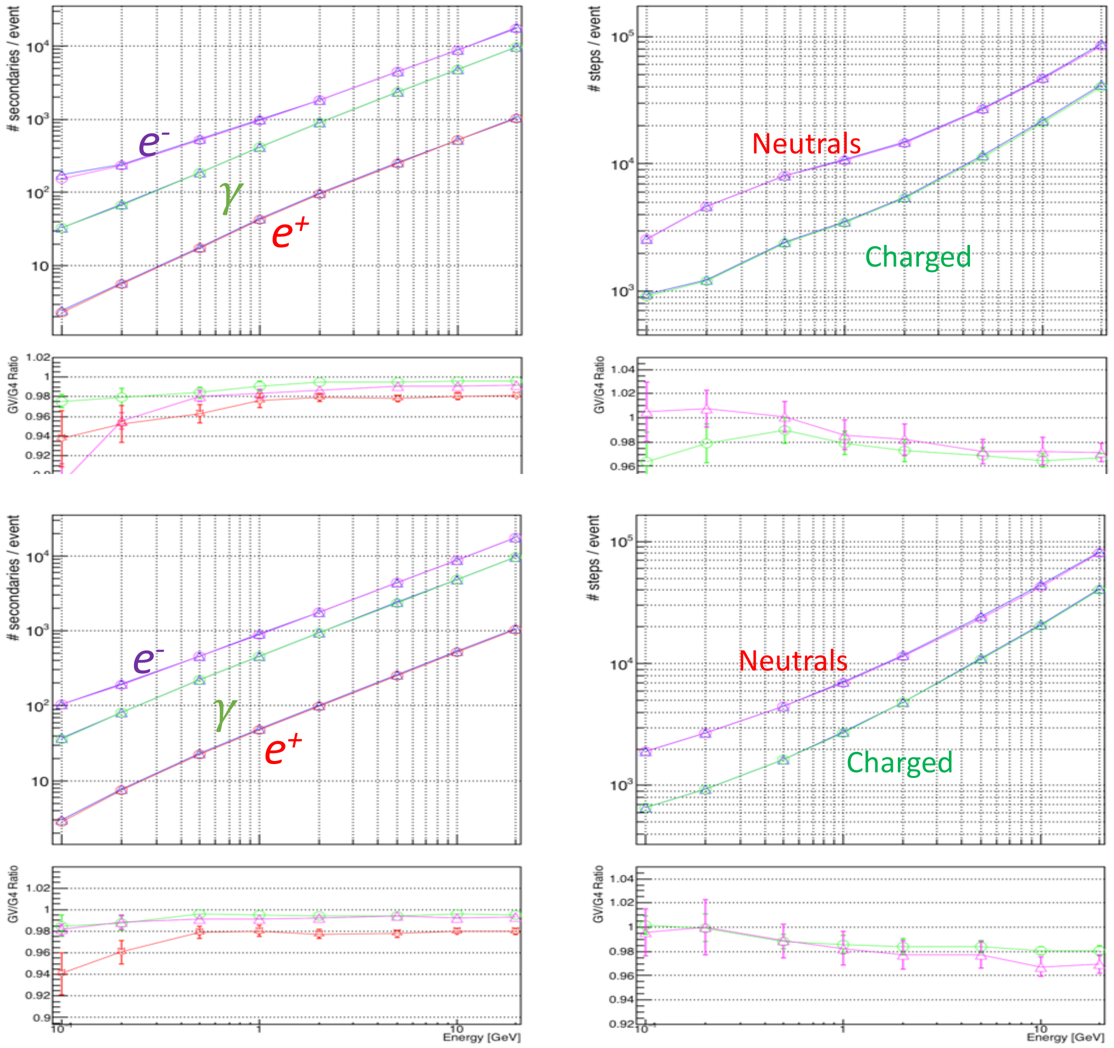
Getting same results for same simulation (2)



- Some ~1% systematics visible in magnetic field
  - Known issue due to difference in tracking/boundary crossing between GeantV and Geant4

CMS example comparisons

- Configuration details: GeantV vs. Geant4 10.04.p03
  - FullCMS geometry (cms.gdml)
  - No field/Map-based magnetic field
  - GeantV-defined physics lists
  - Input: 10 jobs x 1000 *e+* each
- Jobs run on single-thread, scalar mode
- Observables:
  - number of secondaries
  - number of steps
  - track length
- % level mismatches in field, understood



Geant4: blue
GeantV: non-blue

CMS example: stepping observables

B = 0

10^4, 200 [GeV] e- in CMS detector into dir=[0.109764, 0.987878, 0.109764] with exact CMS regions(cuts)

	e^-, e^+ and γ interactions; Magnetic Field: NO	
Mean values per primary	**Geant4**	**GeantV**
total energy deposit:	200 [GeV]	200 [GeV]
total (charged) track length:	198.09 ± 2.72 [m]	197.92 ± 2.98 [m]
total (neutral) track length:	2285 ± 100 [m]	2222 ± 108 [m]
number of (charged) steps:	$4.102\times10^5 \pm 4.914\times10^4$	$4.024\times10^5 \pm 4.999 \times10^4$
number of (neutral) steps:	$7.242\times10^5 \pm 1.18\times10^4$	$6.994\times10^5 \pm 1.208\times10^4$
number of secondary γ:	$9.78\times10^4 \pm 311$	$9.73\times10^4 \pm 321$
number of secondary e^-:	$1.739\times10^5 \pm 1481$	$1.727\times10^5 \pm 1574$
number of secondary e^+:	$1.083\times10^4 \pm 79.32$	$1.061\times10^4 \pm 79.69$

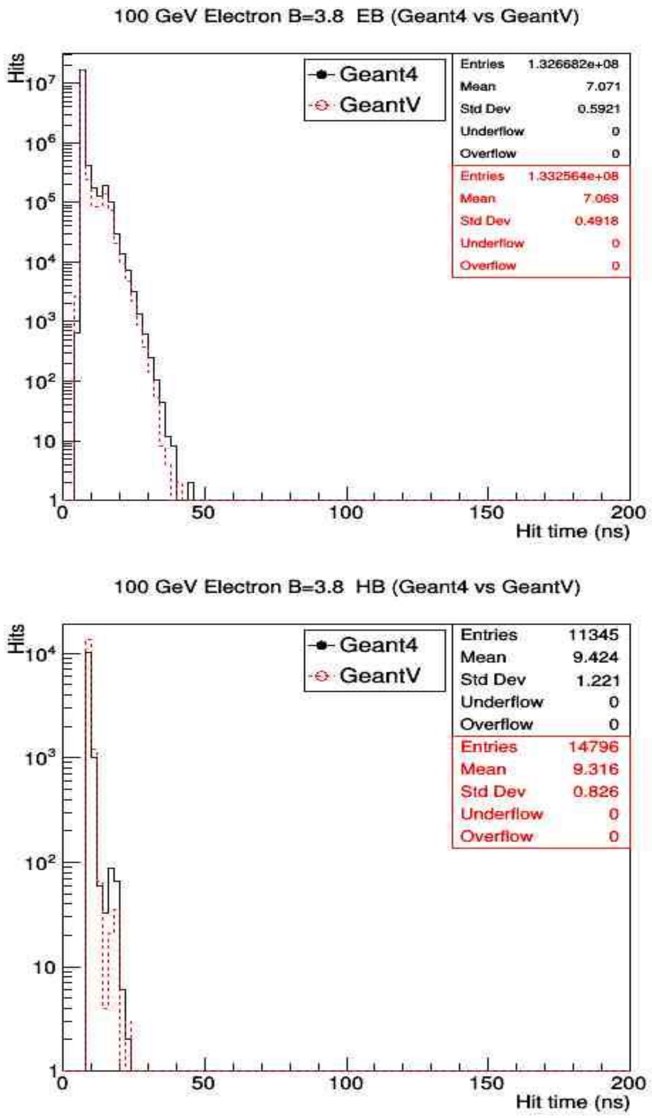
B = 3.8 T

10^4, 200 [GeV] e- in CMS detector into dir=[0.109764, 0.987878, 0.109764] with exact CMS regions(cuts)

	e^-, e^+ and γ interactions; Magnetic Field: 3.8 [T]	
Mean values per primary	**Geant4**	**GeantV**
total energy deposit:	200 [GeV]	200 [GeV]
total (charged) track length:	199.68 ± 6.11 [m]	198.94 ± 6.25 [m]
total (neutral) track length:	2328.25 ± 108 [m]	2260.64 ± 101 [m]
number of (charged) steps:	$4.253\times10^5 \pm 8.128\times10^4$	$4.126\times10^5 \pm 7.644 \times10^4$
number of (neutral) steps:	$7.729\times10^5 \pm 1.605\times10^4$	$7.471\times10^5 \pm 1.5488\times10^4$
number of secondary γ:	$9.78\times10^4 \pm 311$	$9.73\times10^4 \pm 293$
number of secondary e^-:	$1.739\times10^5 \pm 1475$	$1.726\times10^5 \pm 1397$
number of secondary e^+:	$1.083\times10^4 \pm 80.6$	$1.061\times10^4 \pm 75.3$

Physics validation in CMSSW standalone test

- Geant4 10.4p2 w/ VecGeom v0.5 (scalar) vs GeantV pre-beta-7 w/ VecGeom v1.1
  - All CMS-specific G4 optimizations disabled
  - Same production cuts (default 1mm)
  - Single thread (reproducible pRNG sequences)
- Roughly the same distributions with no magnetic field
- Small difference in the physics results in the presence of constant B-field



Hit Time for 100 GeV e- (B=3.8)

Basketizing: efficiency, vectorization, overhead per stage

- Several execution modes to measure stage performance
  - Scalar mode (no baskets): T_{scalar}
  - Vector mode (fill baskets and call vector algorithm): T_{vector}
  - Basket "emulation" mode* (fill baskets and call scalar algorithm in loop): T_{BE}
  - Scalar dispatch mode+ (execute full stepping loop with single particle): T_{SD} -> measure impact of improved GeantV caching

- Measure efficiency & overhead for basketization relative to total run time
  - Overhead: $B_o = (T_{BE} - T_{scalar}) / T_{scalar}$
  - Observed efficiency: $B_e = (T_{scalar} - T_{vector}) / T_{scalar}$
  - Vectorization efficiency: $B_v = B_e + B_o$

** BE mode hard to measure for some stages (e.g. physics) missing emulation of scalar scatter of internal SOA basket*

+ emulating Geant4 stepping but with GeantV data model

Results: basketizing efficiency

CMS application benchmark

- 100 GeV isotropic e^-
- 100 primaries
- Field type: CMS map
- 1 thread, performance mode

Fractions of total scalar execution time

Xeon®CPU E5-2630 v3@2.4 GHz

Stage	% total	B_e	B_o	B_v
Field	14.4%	5.0%	2.0%	7.0%
Phys$^+$	9.4%	0.3%	1.4%	1.7%
Geom*	12.3%	**-3.3%**	3.7%	0.4%
MSC^x	8.6%	1.8%	0.2%	2.0%
FPM^o	32.4%	5.8%	1.5%	7.3%

+ Only post step sampling of physics models
** Only querying distance to boundary and safety*
x Only MSC position/direction correction calculation
o Best configuration for vectorization (Field /Physics/MSC)

Measurement errors < 0.5%

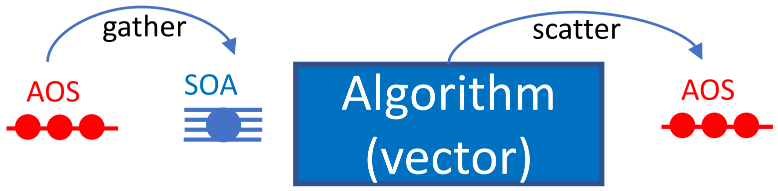
Basketizing overheads dependence on architecture

Geant4 (10.4.p03) vs. GeantV (beta)
10 GeV electron x 1000 events (1-thread, 10 measurements)

CPU	OS	gcc	SIMD	Cache L1	Cache L2	Cache L3	B_o (field)	B_o (physics)	B_o (geometry)	B_o (FPM)
Intel i7 2.5GHz	Ubuntu 16.04	5.4.0	AVX2	126KB	1MB	8 MB	2% ± 1%	2% ± 1%	6% ± 1%	3% ± 1%
Intel Core i7-4510U 2GHz	Ubuntu 16.04	5.4.0	AVX	128KB	512KB	4 MB	-1% ± 7%	-3% ± 7%	12% ± 9%	2% ± 8%
AMD A10-7700k	Fedora Workstation 29	8.2.1	AVX	2x96 KB I 4x16 KB D	2x2M	-	15% ± 1%	4% ± 1%	15% ± 1%	13% ± 1%
Intel R 1.8GHz	Fedora Workstation 29	8.3.1	SSE4	64KB	512KB	2 MB	9% ± 1%	5% ± 1%	9% ± 1%	9% ± 1%

Overhead seems to largely increase for smaller L1 cache size

“Basketizing”: benefits vs. costs



- Costs (coming from initial scalar approach):
  - Workflow redesign, interface redesign, data structure re-engineering
  - Copy overheads: data regrouping, gather/scatter
  - Filling baskets concurrently -> additional overheads due to contention
  - Algorithm vectorization effort
- Benefits:
  - Improved instruction locality
  - Data locality can improve if re-basketizing is done only with collocated tracks
  - SIMD instructions: making use of important % of the silicon for more algorithms
  - Code more compact/efficient and accelerator-ready
- Efficient basketization needs reasonable FLOPS workload
  - Algorithm vectorization can be inefficient for the same reasons as loop vectorization…
    - Branching, early returns, <u>complexity</u>

Performance summary table: Geant4 vs. GeantV

Geant4 (10.4.p03) vs. GeantV (beta)

10 GeV electron x 1000 events (1-thread, 10 measurements)

strk (single track mode): emulation of Geant4 style tracking

Summary of speed-ups for different architectures

CPU	OS	gcc	SIMD	Cache L1	Cache L2	Cache L3	GV [sec]	G4/GV	strk/GV0	Vector Gain
Intel i7 2.5GHz	Ubuntu 16.04	5.4.0	AVX2	126KB	1MB	8 MB	941 ± 6	1.41 ± 0.04	1.00 ± 0.0	1.09 ± 0.01
Intel Core i7-4510U 2GHz	Ubuntu 16.04	5.4.0	AVX	128KB	512KB	4 MB	1,303 ± 6	1.09 ± 0.01	0.95 ± 0.07	1.09 ± 0.08
AMD A10-7700k	Fedora Workstation 29	8.2.1	AVX	2x96 KB I 4x16 KB D	2x2M	-	1,828 ± 6	1.80 ± 0.04	1.00 ± 0.01	1.01 ± 0.01
? Intel R 1.8GHz	Fedora Workstation 29	8.3.1	SSE4	64KB	512KB	2 MB	2,769 ± 6	1.03 ± 0.01	1.00 ± 0.01	0.84 ± 0.01
Intel Centrino2	Fedora Workstation 29	8.2.1	AVX	-	2x2 MB	-	2,592 ± 6	1.92 ± 0.01	1.00 ± 0.01	1.01 ± 0.01
11AMD e-300	Ubuntu 18.10	8.2.0	SSE2	64KB	1 MB	-	Not Vc compatible	Not Vc compatible	1.00 ± 0.01	Not Vc compatible

Is this correctly measured?

CPU performance of G4/GV varies significantly over different platforms

Some open questions

- Single track mode emulating Geant4-like stepping shows very little apparent locality loss (< 10%). Possible reasons:
  - More compact code -> harder to miss the instruction cache
  - Data cache misses are dominant in GeantV, minimizing the effect
- Wildly varying performance ratio GV/G4 depending on architecture, cache configuration
  - Coming from Geant4 being frontend-bound?
  - Cache size/architecture, but also memory latency/throughput?

CPU Benchmark on the Fermilab Wilson Cluster

- Benchmark
  - GeantV (pre-beta-7) vs. Geant4 (10.5)
  - The standalone Geant4/GeantV application using a CMS gdml with a CMS field map
  - 10×10 GeV e−/event, 1000 events
  - measurements on quiet batch nodes (error < 1%)
- CPU Time in [sec] and performance comparisons between Geant4 and Geant4
  - CPU performance widely varies on different processors
  - marginal gain by SIMD vectorization (maximum $\sim$ 10%)

Processor	GeantV	GeantV-vec	Geant4	G4/GV	G4/GV-vec
AVX-2.0-15	2621	2331	4938	1.88	2.12
AVX2-2.4-35	1628	1530	2182	1.34	1.43
SSE4-2.3-15	4457	4333	6627	1.49	1.53

  - Processor: SIMD-CPU[GHz]-Cache[MB]
- What is the source of gain (~1.4-2.1) in Geant4/GeantV?

Vector Instruction and Gain (AVX)

- % of vectorization = (PAPI_DP_VEC)/(PAPI_DP_OPS)
  - PAPI DP VEC = Double precision vector/SIMD instructions
  - PAPI DP OPS = Floating point (double precision) operations
- PAPI (performance API) hardware counters in [1 Billion]

Mode	PAPI_DP_OPS	PAPI_DP_VEC	% vectorization	CPU gain
scalar	1770	277	15.67	-
vec-geo	1771	333	18.82	0.96
vec-mag	1858	814	43.83	1.08
vec-msc	1789	397	22.24	1.02
vec-phys	1785	343	19.25	1.00
vec-all	1868	1051	56.26	1.00
vec-opt	1868	996	53.35	1.12

- % of vectorization is high, but gain is small
  - Vectorization comes with the price of too many data moves and conditional branches

Performance Comparison: Geant4 vs. GeantV libraries

- Exclusive time (%) of big libraries

GeantV Library (%)	AVX	AVX2	SSE4
libGeant_v.so	42.1	46.3	43.2
libRealPhysics.so	36.0	34.2	37.3
libGeantExamplesRP.so	14.1	14.1	14.5
libc-2.12.so	3.8	1.8	1.1
libVmagfield.so	3.1	2.8	3.1
libm-2.12.so	0.6	0.6	0.6
libCore.so	0.1	0.1	0.1
libGeom.so	0.1	0.1	0.1

Geant4 Library (%)	AVX	AVX2	SSE4
libG4geometry.so	41.8	43.6	42.3
libG4processes.so	22.0	20.8	21.0
libG4global.so	7.3	8.0	7.5
libG4tracking.so	7.3	6.5	7.2
libG4track.so	6.0	4.7	5.8
full_cms	5.2	6.1	6.6
libG4clhep.so	3.3	3.0	3.0
libm-2.12.so	2.7	3.5	2.9

- There are no much variations in the percent of time over different processors (CPUs/Cache Size)
- The performance difference between Geant4 and GeantV is a global effect (i.e., not driven by a single module or a set of functions)

Performance Comparison: L1 Cache and TLB Misses

- L1 cache miss: in [Billion] counters

Processor	GV (ICM)	G4(ICM)	GV (DCM)	G4(DCM)
AVX-2.0-15	48	398	190	250
AVX2-2.4-35	48	462	194	248
SSE4-2.3-15	100	285	282	134

  - ICM (DCM) = Instruction (data) cache miss
  - GeantV shows much significantly less ICM
- TLB (translation lookaside buffer) miss: in [1M] counters
  - cache for page tables which map addresses between virtual and physical memory
  - GeantV show much less TLB misses

Processor	GV (IM)	G4(IM)	GV (DM)	G4(DM)
AVX-2.0-15	53	4256	3168	4626
AVX2-2.4-35	N/A	N/A	24	82
SSE4-2.3-15	55	149	88	1628

Performance Comparison: IPC and FMO

- IPC = Instruction(INS)/Cycle(CYC) : Good Balance with Minimal Stall

Processor	GV INS/CYC	GV IPC	G4 INS/CYC	G4 IPC
AVX-2.0-15	7209/6846	1.05	8388/10788	0.78
AVX2-2.4-35	6733/5544	1.21	8458/6178	1.37
SSE4-2.3-15	7847/8869	0.88	8459/11228	0.75

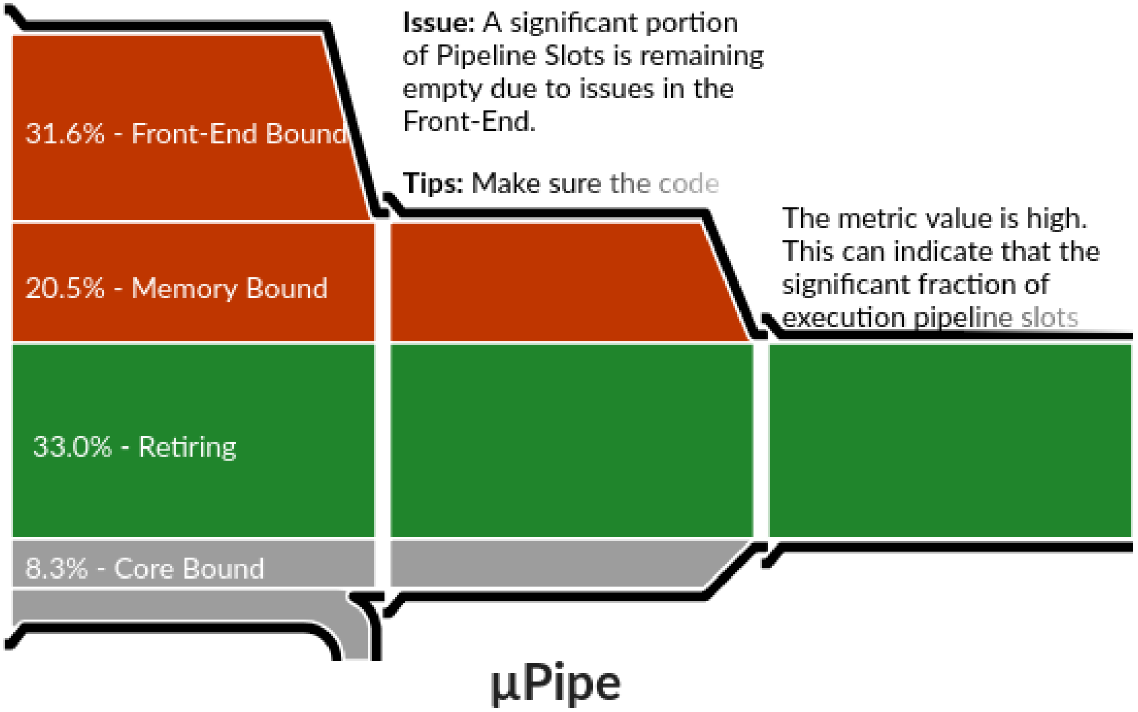
  - ICM (DCM) = Instruction (data) cache miss in [1B] counters
  - GeantV shows significantly less ICM

- FMO = FL/(LD+SR) : CPU Utilization
  - FL (Floating point instruction), LD (load), SR (store) in [1B] counters
  - GeantV shows the better FMO in all tested platforms

Processor	GV FL/(LD+SR)	FMO	G4 FL/(LD+SR)	FMO
AVX-2.0-15	1718/(2422+980)	0.50	2181/(3812+1697)	0.40
AVX2-2.4-35	2347/(882+876)	1.34	3824/(1704+1396)	1.23
SSE4-2.3-15	3191/(1756+1948)	0.86	1620/(1397+4118)	0.29

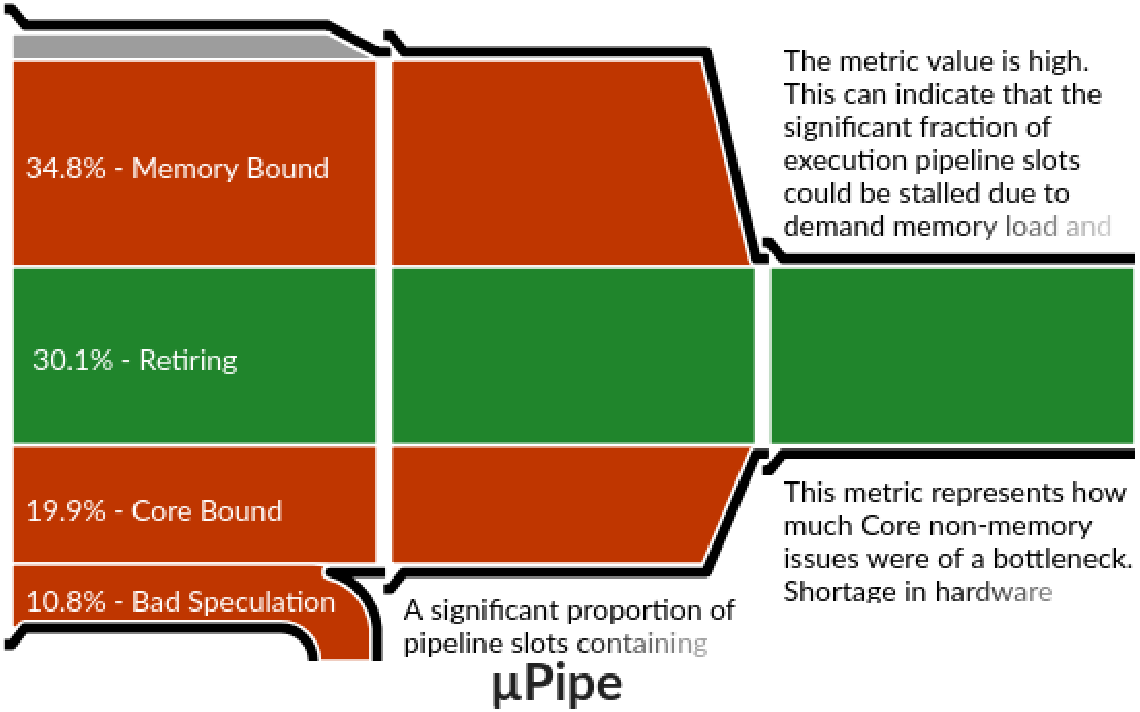
Application profiles from VTune microarchitecture analysis – CMS benchmark

Geant4



Frontend & memory bound

GeantV



Core & memory bound

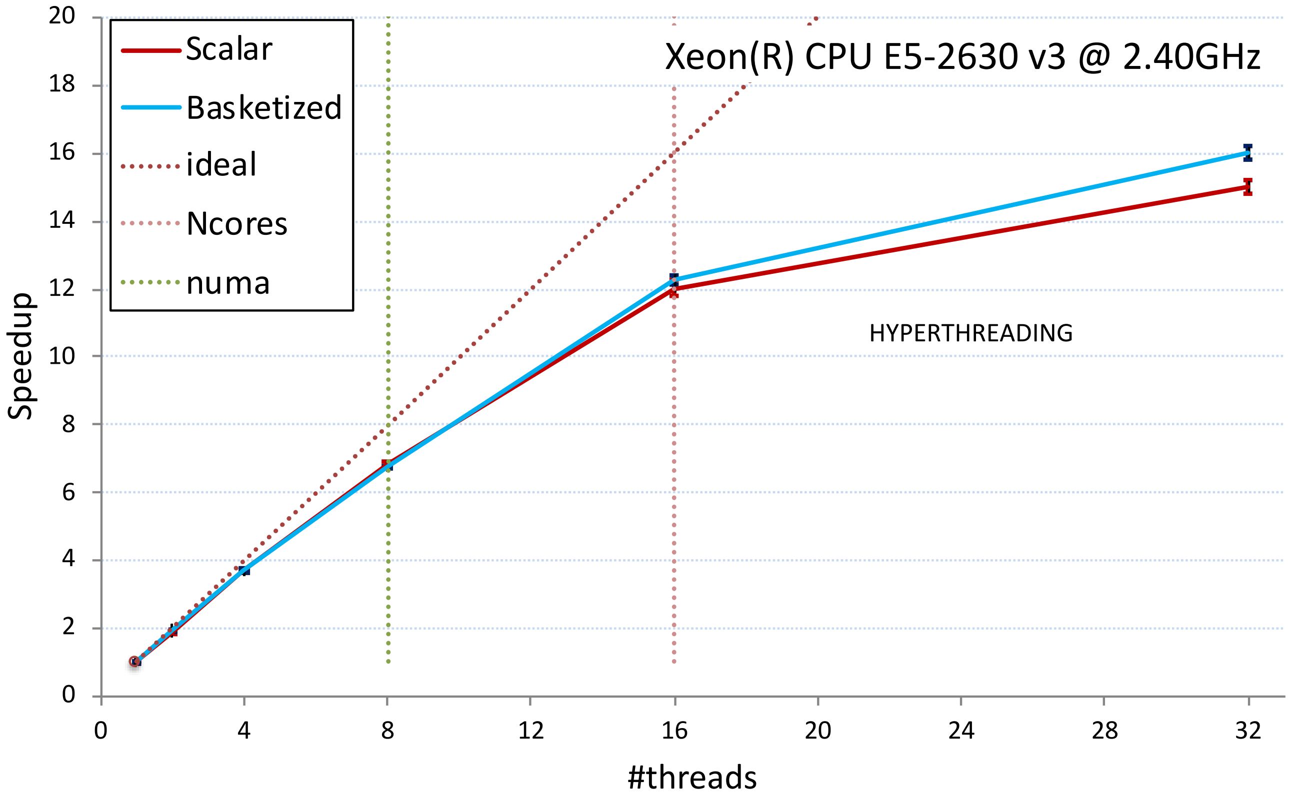
Performance tests for CMSSW integrated example

- Settings:
  - GeantV pre-beta-7+ (63468c9b)
    - Enabled: vectorized multiple scattering, field (not physics)
  - Disable output
- Machine: FermiCloud VM w/ Other machines here?
  - Intel(R) Xeon(R) CPU E5-2660 v2 @ 2.20GHz, 4096 KB cache, sse4.2 instructions
- Standalone GV/G4 test: 2.14× speedup
- CMSSW GV/G4 test: 2.6× speedup with single thread
  - But G4 has better scaling w/ # threads than GV

Concurrency: Strong scaling

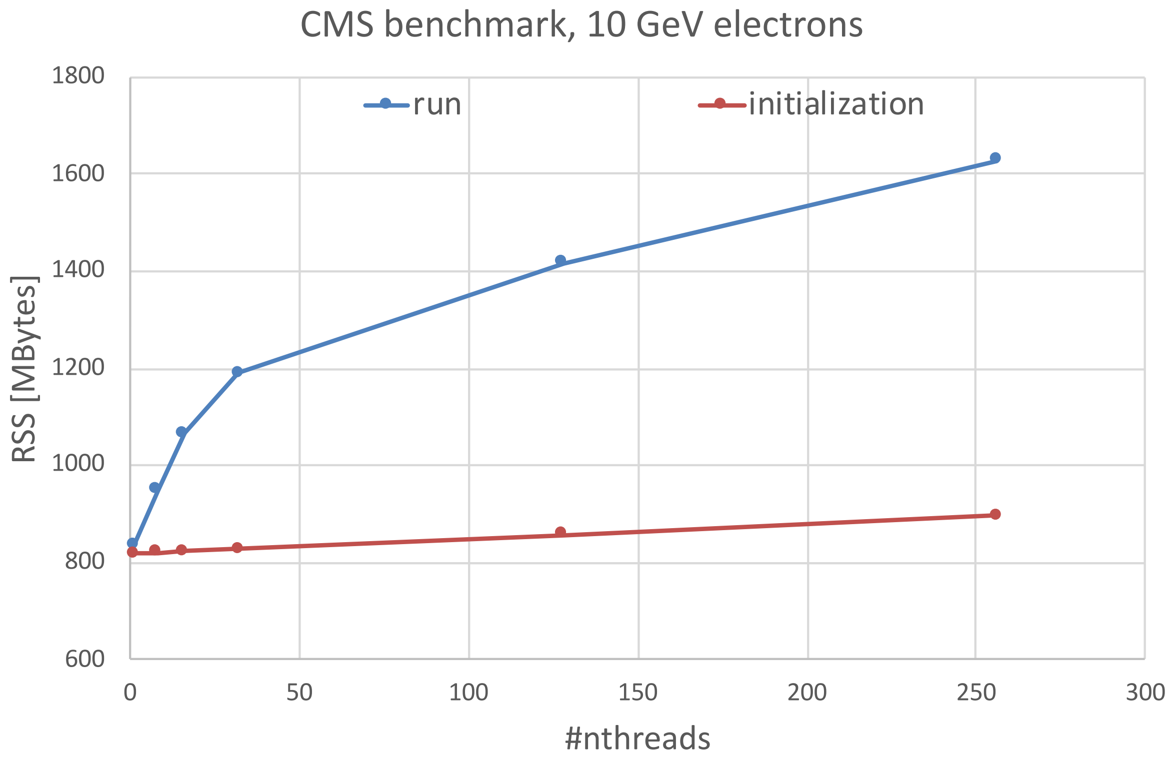
- Acceptable, but far from perfect (~80% efficiency for 16 threads)
  - Price to pay for concurrent services, track stealing
  - Hard to improve w/o fully binding events to threads
- Do we need to exchange tracks between threads?
  - If yes, rather exchange sub-event/track partition than random tracks…

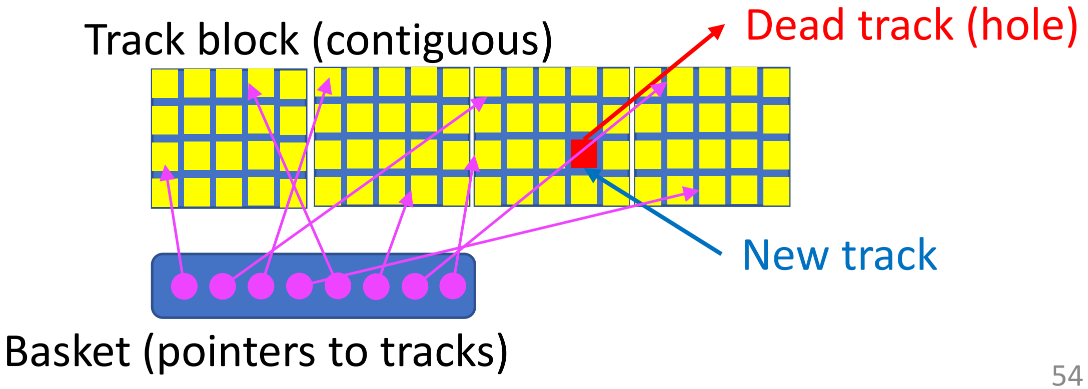
Not just Amdahl, but also basket efficiency loss with #threads



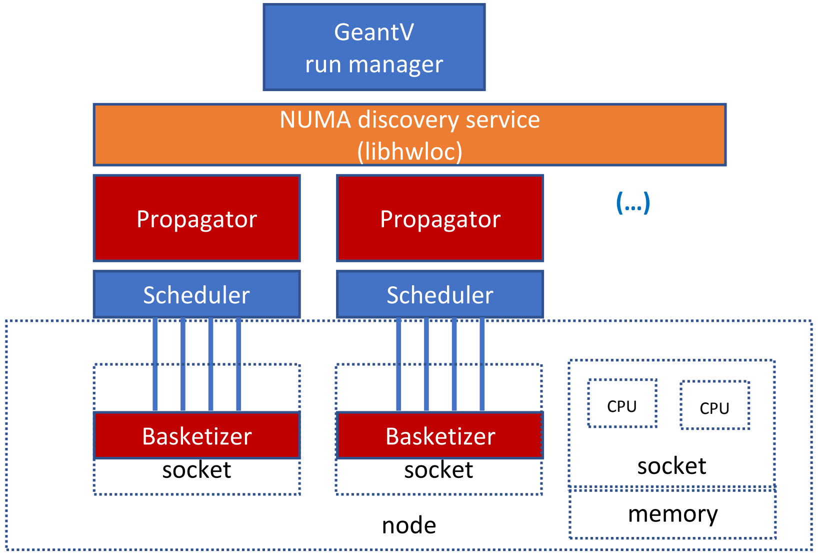
Memory efficiency

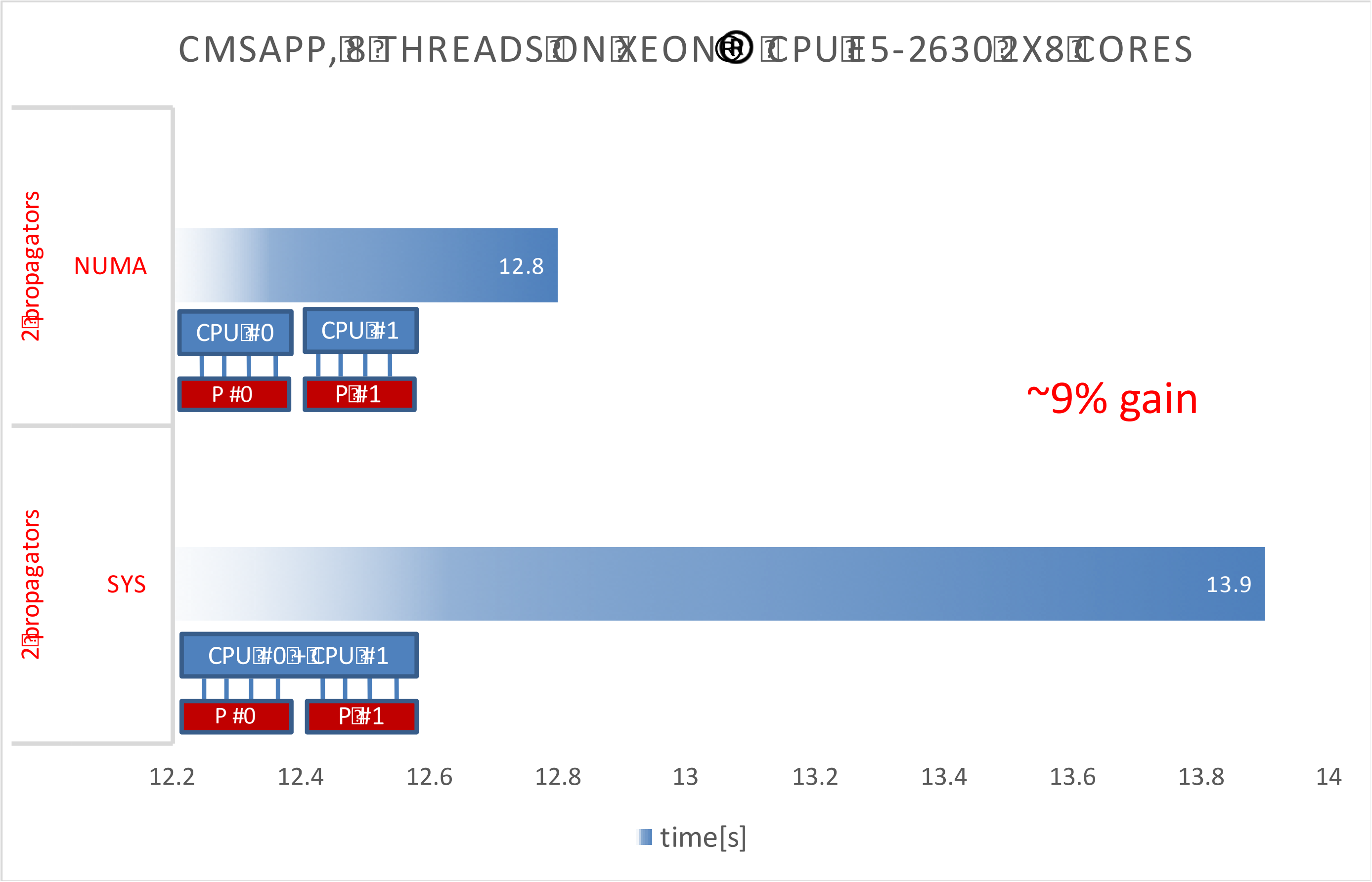
- Larger memory footprint than Geant4 (~3x)
  - Expected to improve for large #nthreads (no study yet)
  - Depending on number of buffered events
- Memory efficiency
  - Scaling with number of tracks in flight
  - Price to pay: baskets not having memory locality -> data cache misses increasing with #nthreads





Topology awareness





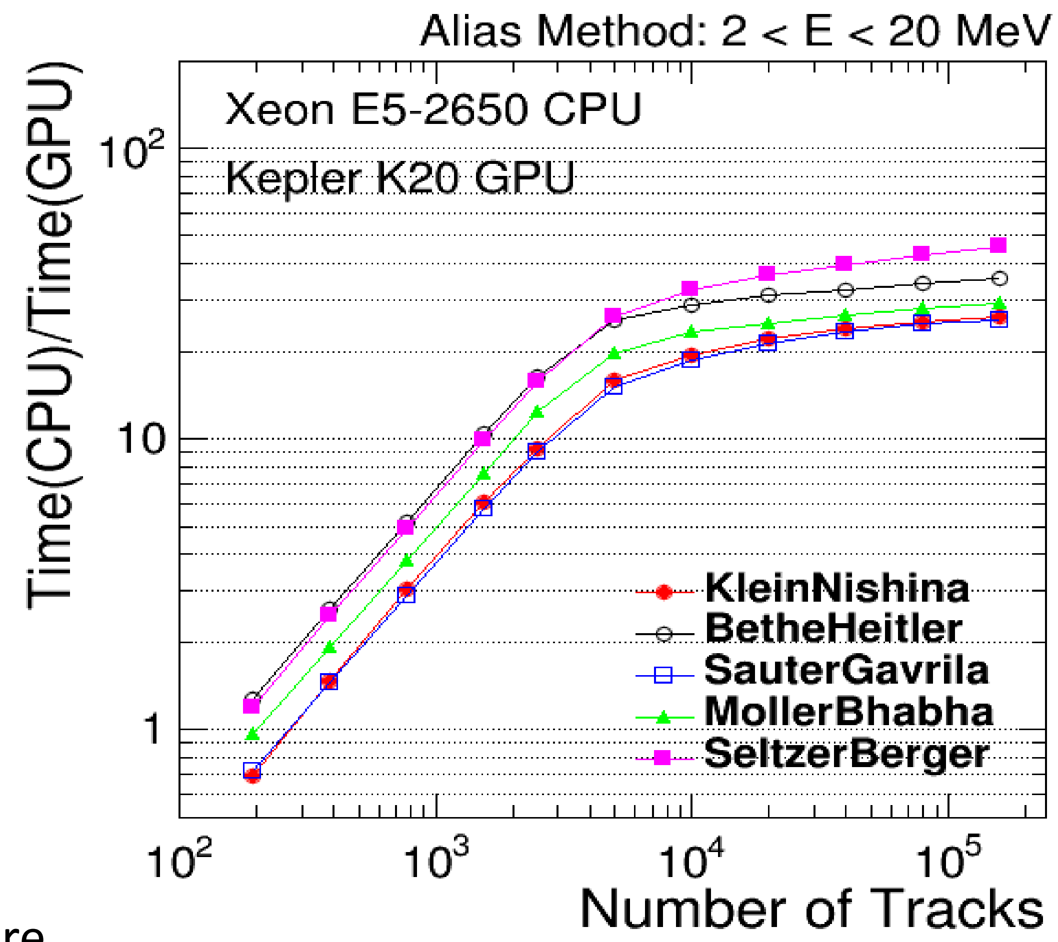
- Thread binding to cores by policy
    - Compact/scatter over NUMA domains
    - Multiple propagators/schedulers
- Track block allocator NUMA aware
    - Blocks owned by threads
- Measurable NUMA effect
    - pointing to data cache misses

Accelerators: integration with the "basket" model

- Portability: CUDA as a backend

- GPU baskets and performance
  - CPU Intel Xeon E5 (1 core @2.6GHz)
  - NVidia K20 GPU (2096 cores @0.7GHz)
  - EM models (sampling final states)
  - Performance as the number of tracks
  - Potential of *x30* on GPU, but requires *10^4* tracks per process

- Lessons:
  - Portability is feasible, but does not come for free
  - efficiency comes with very large baskets, which are difficult to maintain



Concurrency lessons

- The more thread-local the data flow the better
  - Keep tracks in the same thread, with minimum stealing
  - Avoid high contention on common data containers
    - Concurrent basketizing has high price, some baskets had to become thread local
- A MT multi-basketized flow becomes inefficient on event tails
  - Partial baskets have to be flushed in scalar mode to sustain the data flow
- Track-level parallelism cuts event tails, but has large price
  - Multiple events in flight, but owned by a thread - is it a good compromise?
  - Track-level parallelism is the path to instruction-level parallelism

6. Lessons learnt

How could it be done better?

Open questions

- Still not fully understanding all sources of performance increase of GeantV
  - Would need extra time/resources/expertise
- Sharing tracks opens up fine grain parallelism, but extra communication hinders on performance: what is the best trade-off?
- How to improve both instruction and data locality, is it even possible?
  - Needs rethinking the data model and access patterns

Main lessons (1)

- Main factors in the speedup seem to include
  - Better cache use
  - Tighter code (e.g., less indirections and branching)
- Vectorization’s impact (much) smaller than hoped for
  - Basketization can bring benefits for FP hotspots (e.g. magnetic field, multiple scattering
  - Small fraction of the code has been vectorized or is run in vector mode effectively
  - Overhead of per volume basketization cost similar to vector gain for “small” modules
- Basketization cost in
  - Either extra memory copy (using collection of tracks)
  - Or lower memory access coherency (using collection of pointers)

Main lessons (2)

- Geometry navigation not (yet?) vectorized and introduces a bottleneck (Amdahl)
    - Mainly due to the end-of-event track collection/gathering from the ‘rarely’ used volumes
    - Should decrease for larger track multiplicities
    - But no guarantee that these volumes internally vectorize
- Code/Algorithm needs to be designed from the ground up for vectorization for best results
    - Compact code, compact data fitting caches and being reused
- Actual upper limit on potential vectorization gains are still to be fully understood
    - including whether different approaches and **trade-offs** in the physics code implementation could bring extra computing performance
    - Including AVX512 that was not tested due to not working backends

Conclusions (1)

- Innovative and disruptive R&D allowing to investigate novel technologies and approaches to simulation
  - Allowed to improve performance-critical code in the simulation chain
  - Still more room for improvement
- Showed the significant impact of good CPU cache behavior (and the challenge of measuring this effect)
  - Further research warranted to see if this can be exploited even further
- Basketization gains overshadowed by associated costs mainly due to data copy/management overheads.
  - Nonetheless might still benefit other workflows (e.g. pipelines)
  - Balance might be different under different conditions (e.g. larger multiplicities)

Conclusions (2)

- Amdahl's law applies to vectorization too :(
- Lessons learned will be useful for GPU architecture investigations
- GeantV allowed to venture into interesting and ambitious R&D paths and set new expectations for the future, both in terms of potential gains and the cost of achieving them

Follow-up

- Reusable components and ideas for improving existing Geant4
  - Extending VecCore, VecMath, VecGeom
  - Investigate basketization of few performance-critical components in Geant4
- Follow-up plans
  - Compact specialized libraries as alternative to general stepping approach
  - Extraction of basketization generic library, possible basketization of FP-intensive components
  - Disentangling state from managers and move towards more functional programing style
    - Increase flexibility of functional-based regrouping, enable parallelism opportunities below event level.
  - Review the data model and flow in Geant4 to pre-empt extra parallelism and acceleration opportunities
  - …
- Pere will take care of most of this in his presentation

Thank you!

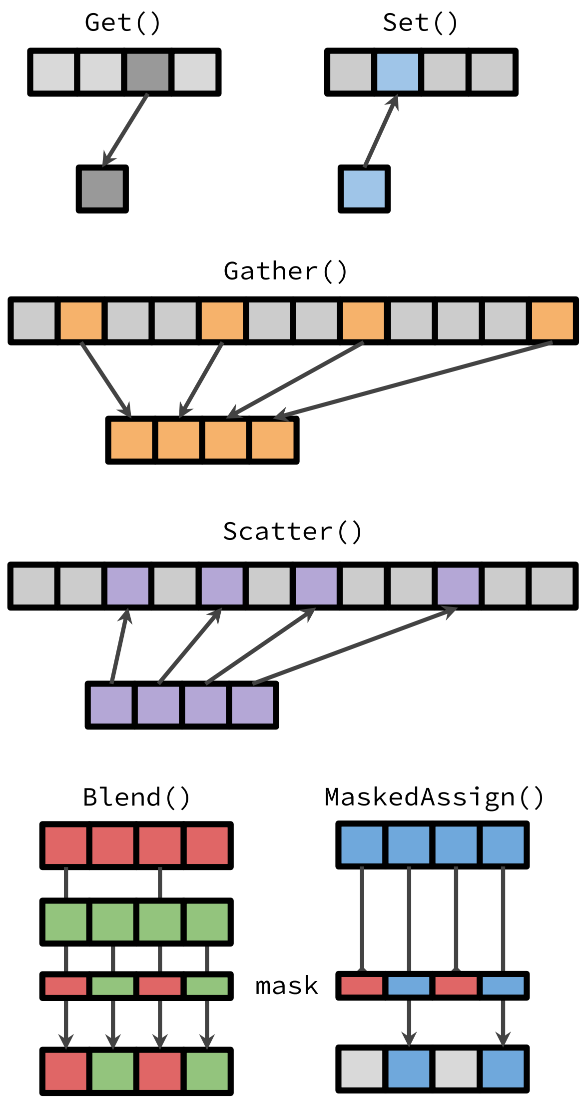
Thanks to all the GeantV collaborators contributing to different parts of this R&D

Backup slides

More detailed info about the different topics

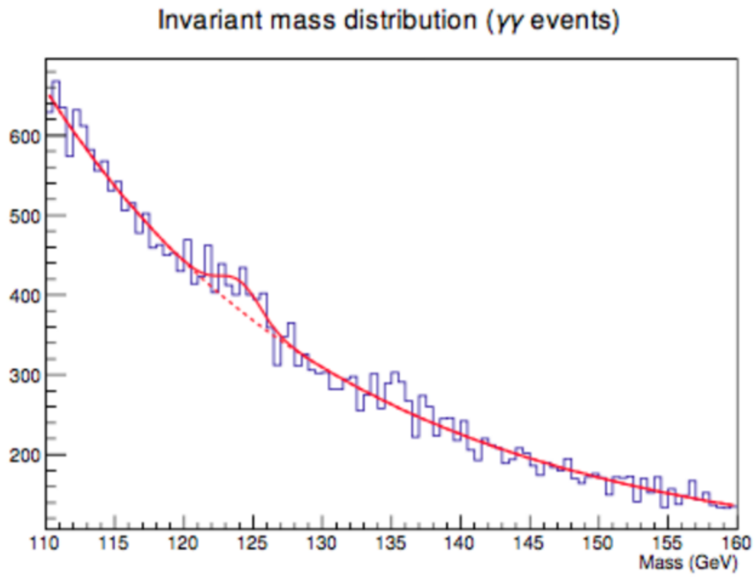
VecCore SIMD Abstraction Library

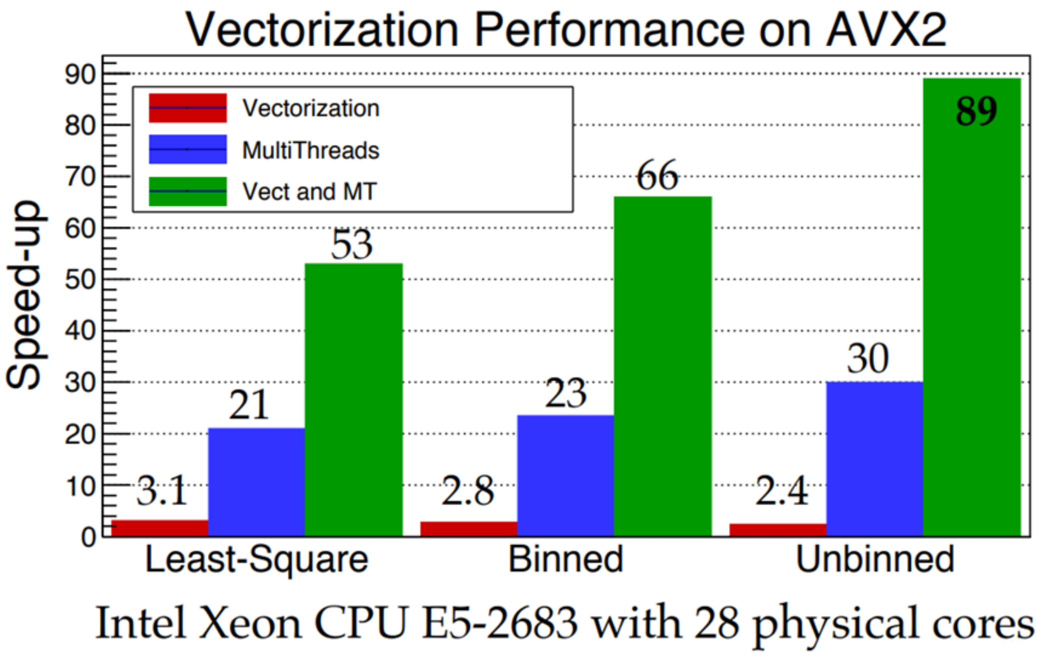
- Simple API abstracting common SIMD operations in a generic way
- Evolution of “backends” from VecGeom
- Became a standalone library in 2017: https://github.com/root-project/veccore
- Used by VecGeom and ROOT
- Supports SIMD in x86_64 via Vc and UME::SIMD, SSE2 to AVX512
- Supports ARM, PPC64 with scalar backend
- Supports Windows, Mac, and Linux



Why use SIMD Vectorization?

SIMD vectorization is already essential for high performance on modern Intel® processors, and its relative importance is expected
to increase, especially on hardware geared towards HPC, such as Xeon Phi™ and Skylake Xeon™ processors.





Vectorization of ROOT Mathematical Libraries — CHEP 2018, Sofia, Bulgaria
Reference: https://indico.cern.ch/event/587955/contributions/2938041/attachments/1683418/2706263/Vectorization_chep2018.pdf

SIMD Programming Models

- Auto-vectorization
- OpenMP 4.1
- Compiler Pragmas
- SIMD Library
- Compiler Intrinsics
- Assembly

```
float a[N], b[N], c[N];

for (int i = 0; i < N; i++)
  a[i] = b[i] * c[i];
```

```
float a[N], b[N], c[N];

#pragma omp simd
#pragma ivdep
for (int i = 0; i < N; i++)
  a[i] = b[i] * c[i];
```

```
#include <Vc/Vc>
Vc::SimdArray<float, N> a, b, c;

a = b * c;
```

```
#include <x86intrin.h>
__m256 a, b, c;

a = _mm256_mul_ps(b, c);
```

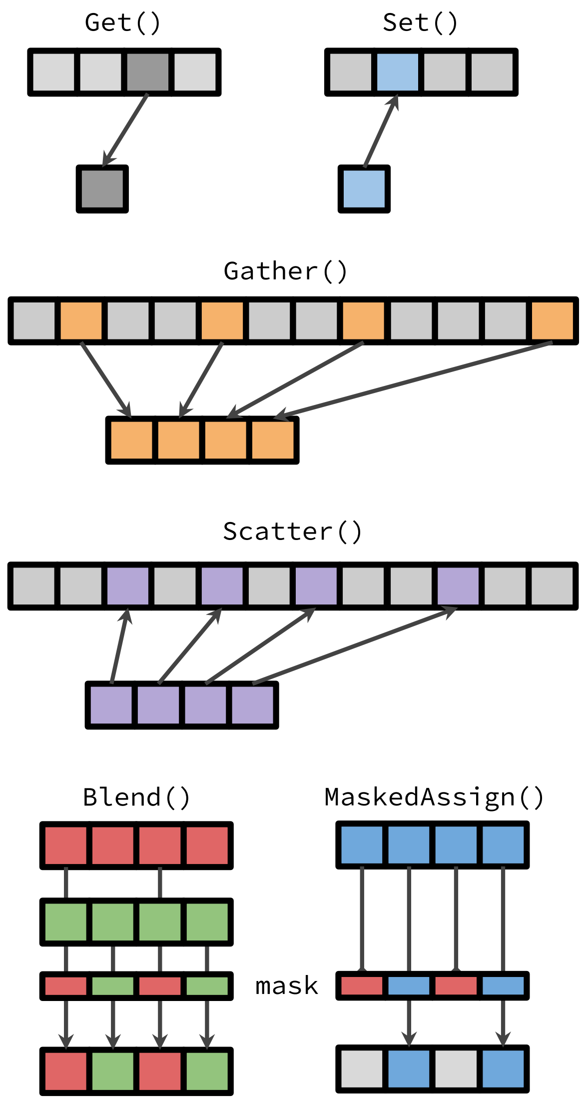
```
asm volatile("vmulps %ymm1, %ymm0");
```

Why did we need VecCore?

- Unreliable performance with auto-vectorization
  - `https://godbolt.org/g/bjQzbA` (change int to bool)
  - `https://godbolt.org/g/R6fXAw` (change -O1 to -O3)
- Compiler intrinsics are not an ideal interface
  - Limited to C name mangling, so portability is an issue
- Libraries do not work well across all architectures
  - UME::SIMD is best on KNL, but Vc is better for Skylake
  - ARM support only in UME::SIMD, but poor performance
- Portable solution for when no library is available
  - For example, on PowerPC

VecCore API

```cpp
namespace vecCore {

  template <typename T> struct TypeTraits;
  template <typename T> using Mask   = typename TypeTraits<T>::MaskType;
  template <typename T> using Index  = typename TypeTraits<T>::IndexType;
  template <typename T> using Scalar = typename TypeTraits<T>::ScalarType;

  // Vector Size
  template <typename T> constexpr size_t VectorSize();

  // Get/Set
  template <typename T> Scalar<T> Get(const T &v, size_t i);
  template <typename T> void Set(T &v, size_t i, Scalar<T> const val);

  // Load/Store
  template <typename T> void Load(T &v, Scalar<T> const *ptr);
  template <typename T> void Store(T const &v, Scalar<T> *ptr);

  // Gather/Scatter
  template <typename T, typename S = Scalar<T>>
  T Gather(S const *ptr, Index<T> const &idx);

  template <typename T, typename S = Scalar<T>>
  void Scatter(T const &v, S *ptr, Index<T> const &idx);

  // Masking/Blending
  template <typename M> bool MaskFull(M const &mask);
  template <typename M> bool MaskEmpty(M const &mask);

  template <typename T>
  void MaskedAssign(T &dst, const Mask<T> &mask, const T &src);

  template <typename T>
  T Blend(const Mask<T> &mask, const T &src1, const T &src2);

} // namespace vecCore
```



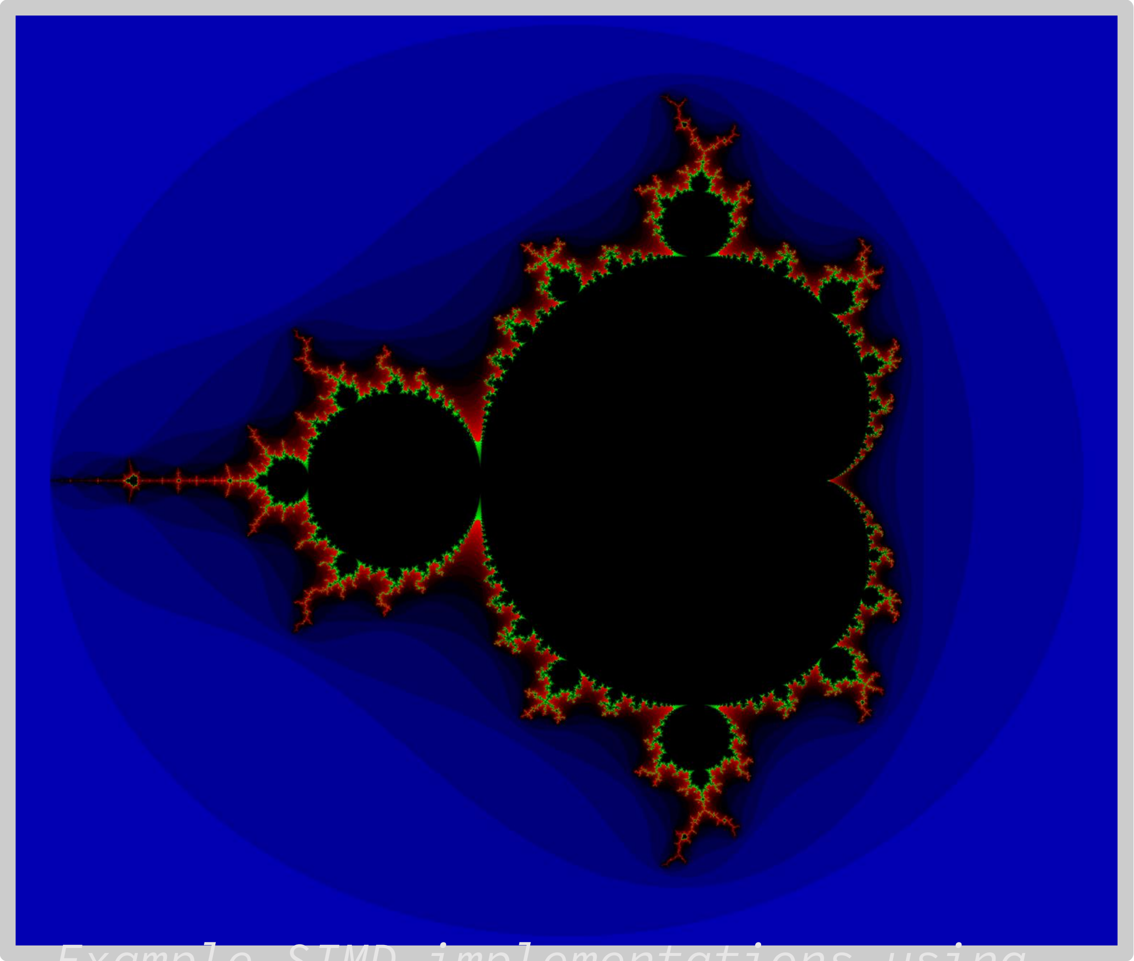
VecCore Example: Mandelbrot Set

Iterate

$$f(z) = z^2 + c$$

N times and check if *z* diverges

Example included in VecCore



`Example SIMD implementations using intrinsics:`

`https://github.com/skeeto/mandel-simd`

`Shows speedup of 5.8x with AVX`

VecCore Example: Mandelbrot Set

Iterate

$f(z) = z^2 + c$

N times and check if *z* diverges

Example included in VecCore

Scalar Implementation

```
template<typename T>
 void mandelbrot(T xmin, T xmax, size_t nx,
                 T ymin, T ymax, size_t ny,
                 size_t max_iter,
                 unsigned char *image)
 {
     T dx = (xmax - xmin) / T(nx);
     T dy = (ymax - ymin) / T(ny);

     for (size_t i = 0; i < nx; ++i) {
         for (size_t j = 0; j < ny; ++j) {
             size_t k = 0;
             T x = xmin + T(i) * dx, cr = x, zr = x;
             T y = ymin + T(j) * dy, ci = y, zi = y;

             do {
                 x  = zr*zr - zi*zi + cr;
                 y  = 2.0 * zr*zi + ci;
                 zr = x;
                 zi = y;
             } while (++k < max_iter &&
                          (zr*zr+zi*zi < 4.0));

             image[ny*i+j] = k;
         }
     }
 }
```

VecCore Example: Mandelbrot Set

Iterate

$f(z) = z^2 + c$

N times and check if *z* diverges

Example included in VecCore

VecCore Implementation

```
template<typename T>
void mandelbrot_v(Scalar<T> xmin, Scalar<T> xmax, size_t nx,
                  Scalar<T> ymin, Scalar<T> ymax, size_t ny,
                  Scalar<Index<T>> max_iter,
                  unsigned char *image)
{
    T iota;
    for (size_t i = 0; i < VectorSize<T>(); ++i)
        Set<T>(iota, i, i);

    T dx = T(xmax - xmin) / T(nx);
    T dy = T(ymax - ymin) / T(ny), dyv = iota * dy;

    for (size_t i = 0; i < nx; ++i) {
        for (size_t j = 0; j < ny; j += VectorSize<T>()) {
            Scalar<Index<T>> k{0};
            T x = xmin + T(i) * dx,      cr = x, zr = x;
            T y = ymin + T(j) * dy + dyv, ci = y, zi = y;

            Index<T> kv{0};
            Mask<T> m{true};

            do {
                x = zr*zr - zi*zi + cr;
                y = T(2.0) * zr*zi + ci;
                MaskedAssign<T>(zr, m, x);
                MaskedAssign<T>(zi, m, y);
                MaskedAssign<Index<T>>(kv, m, ++k);
                m = zr*zr + zi*zi < T(4.0);
            } while (k < max_iter && !MaskEmpty(m));

            for (size_t k = 0; k < VectorSize<T>(); ++k)
                image[ny*i+j+k] = (unsigned char) Get(kv, k);
        }
    }
}
```

Performance of Mandelbrot Set

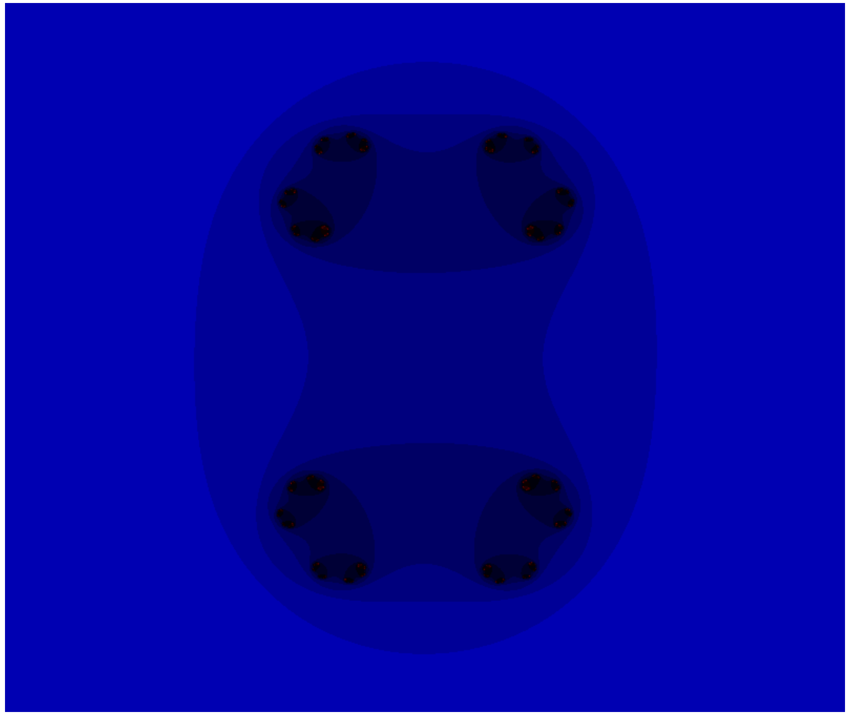
		Intel Core i7 6700			Intel Xeon Phi 7210	
Runtime (ms)		GCC-7.2	Clang-5.0	ICC-18.0	GCC-7.2	ICC-18.0
Single Precision	Scalar	550	549	677	3415	3609
	Scalar Backend	570	569	677	3353	3510
	Vc 1.3.3	110	110	126	1064	1160
	UME::SIMD 0.8.1	117	117	131	–	543
Double Precision	Scalar Algorithm	548	548	672	3409	3602
	Scalar Backend	571	571	674	3348	3502
	Vc 1.3.3	267	267	257	2101	2087
	UME::SIMD 0.8.1	421	421	422	–	846
Speedup vs Scalar						
Single Precision	Scalar Backend	0.96	0.96	1.00	1.02	1.03
	Vc 1.3.3	5.00	4.99	5.37	3.21	3.11
	UME::SIMD 0.8.1	4.70	4.69	5.17	–	6.65
Double Precision	Scalar Backend	0.96	0.96	0.99	1.02	1.03
	Vc 1.3.3	2.05	2.05	2.61	1.72	1.73
	UME::SIMD 0.8.1	1.30	1.30	1.59	–	4.25

Note: "Scalar" above has SSE2 enabled, single precision time with SSE2 disabled with GCC-7.2 is 764ms.

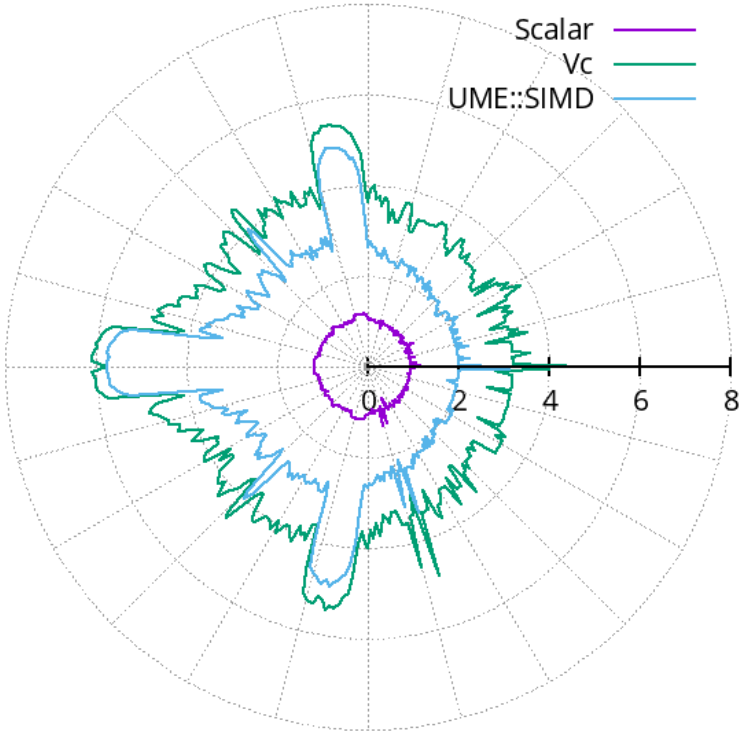
Reference: https://indico.cern.ch/event/567550/papers/2700128/files/6152-

Effect of branching on SIMD performance

Iterate $f(z) = z^2 + c$, where
$c = 0.7885\, e^{i\alpha}$ and $\alpha \in [0, 2\pi]$



Julia Set



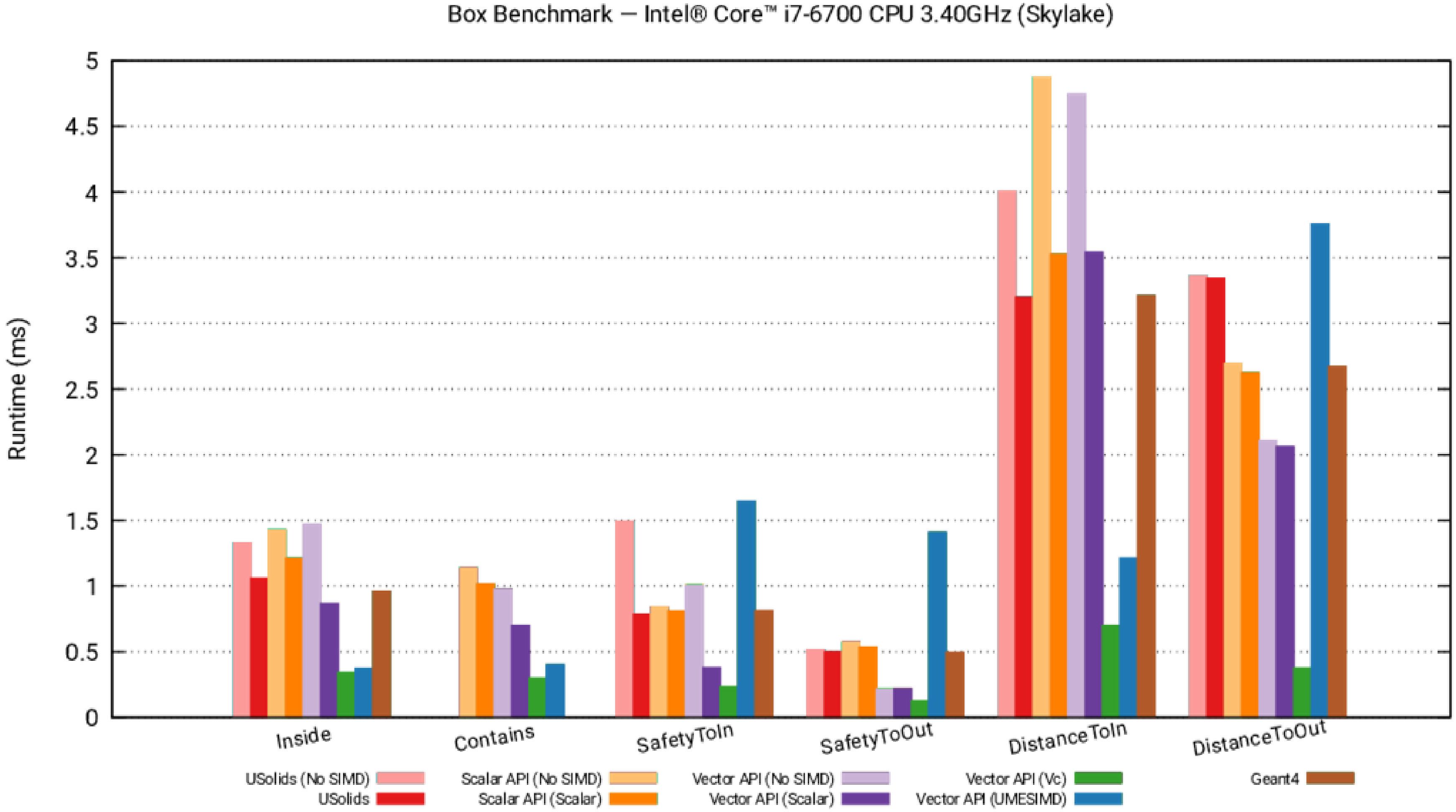
Speedup

Code Sample: VecGeom Box

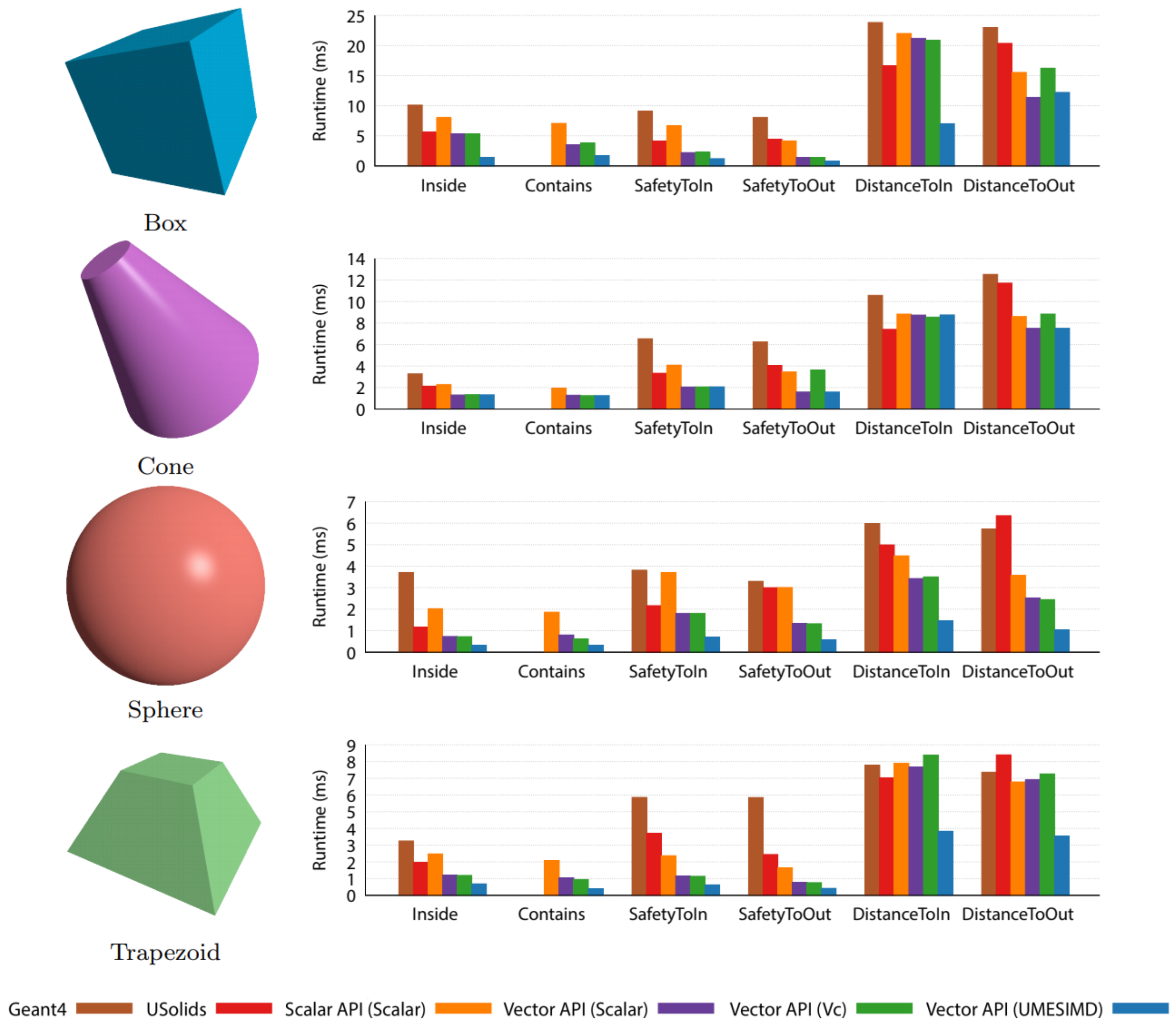
Box Implementation of `DistanceToIn()`

```
template <typename Real_v>
void DistanceToIn(UnplacedStruct_t const &box, Vector3D<Real_v> const &point,
                  Vector3D<Real_v> const &direction, Real_v const &stepMax, Real_v &dist)
 {
   const Vector3D<Real_v> invDir(Real_v(1.0) / NonZero(direction[0]),
                                 Real_v(1.0) / NonZero(direction[1]),
                                 Real_v(1.0) / NonZero(direction[2]));

   const Real_v distIn = Max((-Sign(invDir[0]) * box.fDimensions[0] - point[0]) * invDir[0],
                             (-Sign(invDir[1]) * box.fDimensions[1] - point[1]) * invDir[1],
                             (-Sign(invDir[2]) * box.fDimensions[2] - point[2]) * invDir[2]);

  const Real_v distOut = Min((Sign(invDir[0]) * box.fDimensions[0] - point[0]) * invDir[0],
                             (Sign(invDir[1]) * box.fDimensions[1] - point[1]) * invDir[1],
                             (Sign(invDir[2]) * box.fDimensions[2] - point[2]) * invDir[2]);

   dist = Blend(distIn >= distOut || distOut <= Real_v(kTolerance), Infinity<Real_v>(), distIn);
 }
```

Performance of VecGeom Box Algorithms



VecGeom Speedups on Knights Landing



Field propagation overview

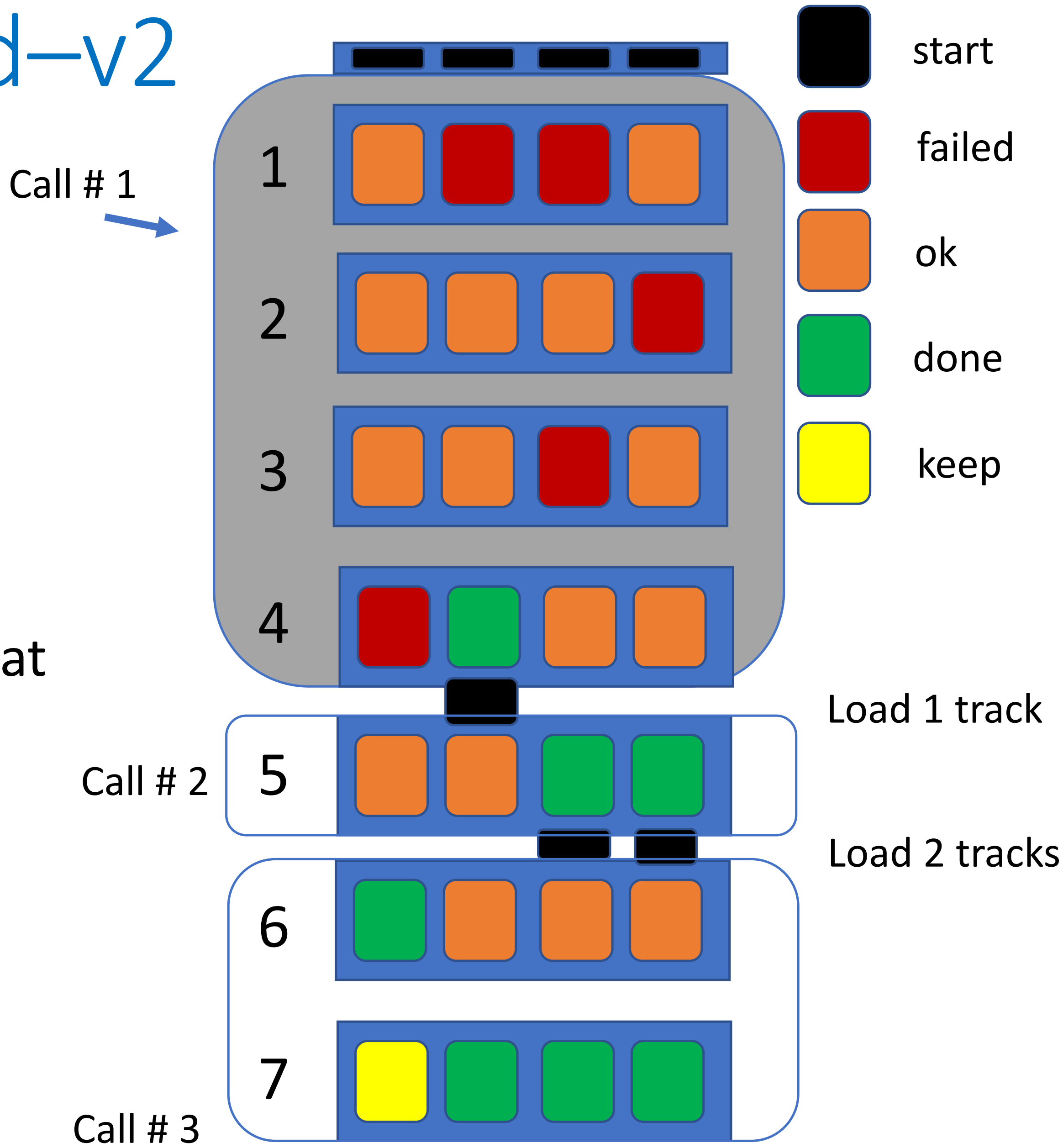
$\mathbf{x}_0, \mathbf{p}_0$
$\mathbf{x}_1, \mathbf{p}_1, \mathbf{\Delta x}, \mathbf{\Delta p}$
$\mathbf{x}_2, \mathbf{p}_2, \mathbf{\Delta x}, \mathbf{\Delta p}$

- Field propagation involves solution of Ordinary Differential Equation
  - Typically Runge-Kutta methods are used (as in Geant4)
- In GeantV created **vectorised Runge-Kutta** propagation
  - Charged tracks in a basket are sent to the FieldPropagation classes
  - Vectorised over tracks
- Challenges are
  - To use mostly vector operations
  - To ensure that all vector lanes are doing useful work

- Motion in field requires solving ODE for endpoint **x**, **p** after length s
- Runge-Kutta step: evaluate B-field, estimate **x**, **p**, **Δx**, **Δp**
- Successful if $|\mathbf{\Delta x}| < \varepsilon\, s$ & $|\mathbf{\Delta p}| < \varepsilon\, |\mathbf{p}|$
- Each step of a Runge-Kutta algorithm is easy to vectorise
  - But different tracks (vector lanes) can take different number of iterations to finish integration
  - The ‘driver’ class which calls the RK ‘stepper’ must play coordinate the work

Vector propagation in Field–v2

- A step can either
  - Fail,
  - Succeed but not get to the end ("ok")
  - Finish the integration ("done")
- Driver rewritten to use
  - Tight loop with all lanes integrating until at n>=threshold reach the end of interval
  - Reload lanes with new work.
- Profiled with (semi-)realistic RZ field
  - Interpolated from sampled CMS field



Performance with baskets for field only

Basket size	16	32	64	128	256	512	1024
Unused lanes	0.186	0.130	0.073	0.039	0.023	0.015	0.007
Unused lanes (reordering)	0.140	0.066	0.025	0.003	0.002	0.001	0.001

Fraction of lanes which have finished integration.

Event window	Tracks/event	Basket sz= 16	32	64	128	256	512	1024
16	16	3.4 (2) %	**5.6 (2) %**	4.0 (2) %	4.1 (2) %	5.2(2) %	3.6 (2) %	1.6 (2) %
1	16		4.7 (2) %	5.0 (2) %	5.5 (2) %	6.8(2) %	**7.0 (3) %**	
1	8 reordering	6.6 (3) %	5.3 (3) %	6.9 (3) %	7.2 (4) %	7.9(4) %	**8.2 (3) %**	7.3(3) %

Benchmarks on 1 thread of *MacBook Pro 2016, 2.6 GHz Core i7 6700HQ (Skylake),* 16 GB LPDDR3 2133MHz RAM, with clang from Xcode 10.1.

Baseline is “Basket off” configuration with 16 event window with 16 tracks/event (10 GeV e-).

‘Reordering’ means bringing forward tracks with length / radius(curvature) over threshold (=1.5)

EM Physics

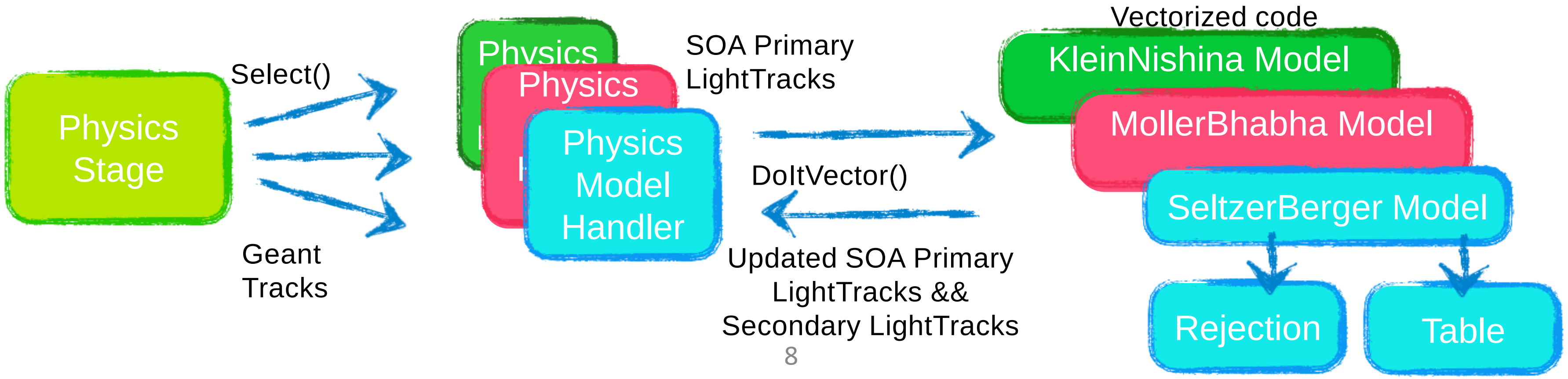
Backup slides

Vectorized EM physics models – Intro

- A **simulation step**, limited by a discrete physics interaction, can be divided into **two** distinct parts
  - **Select the physics interaction** with the corresponding interaction point:
    - Driven by the integrated cross section values of the physics
    - Cross section table lookups and interpolations (Memory bounded operations with very little mathematical computations)
  - **Invoke the interaction** (**final state sampling**):
    - Computation of the post-interaction kinematical state of the primary particle
    - Generation of possible secondary particles
    - Contains significantly more mathematical operations (CPU bounded)
- The **final state computation** includes generation of **stochastic variables** from their probability distributions determined by the corresponding differential (in energy, angle) cross sections (DCS) of the underlying physics interaction
  - **Composition-rejection** method is typically used in Geant4 to sample from these PDFs

Sampling techniques for the Final State generation

- **Rejection Sampling:**
  - Unpredictable n. of loop executions: Exit condition depends on the outcome of the stochastic variable
  - Non deterministic behavior for the different tracks filled into the vector register, resulting in undesired divergence and eventually loss of potential computational gain
  - Solution: lane refilling
- **Table Sampling:**
  - **Alias** method efficiently generates samples of discrete stochastic variables
  - An intermediate **discrete random variable** is introduced by partitioning the range of the original continuous PDFs into distinct intervals
    - new discrete variable is the probability of having the original continuous variable lying in a given interval
  - **Appropriate partitions** of the original variable range and/or **variable transformations** are used to transform the original PDF to a smooth function, in order to have a linear behavior of the PDF over each discrete interval



Vectorized EM physics models

[1]

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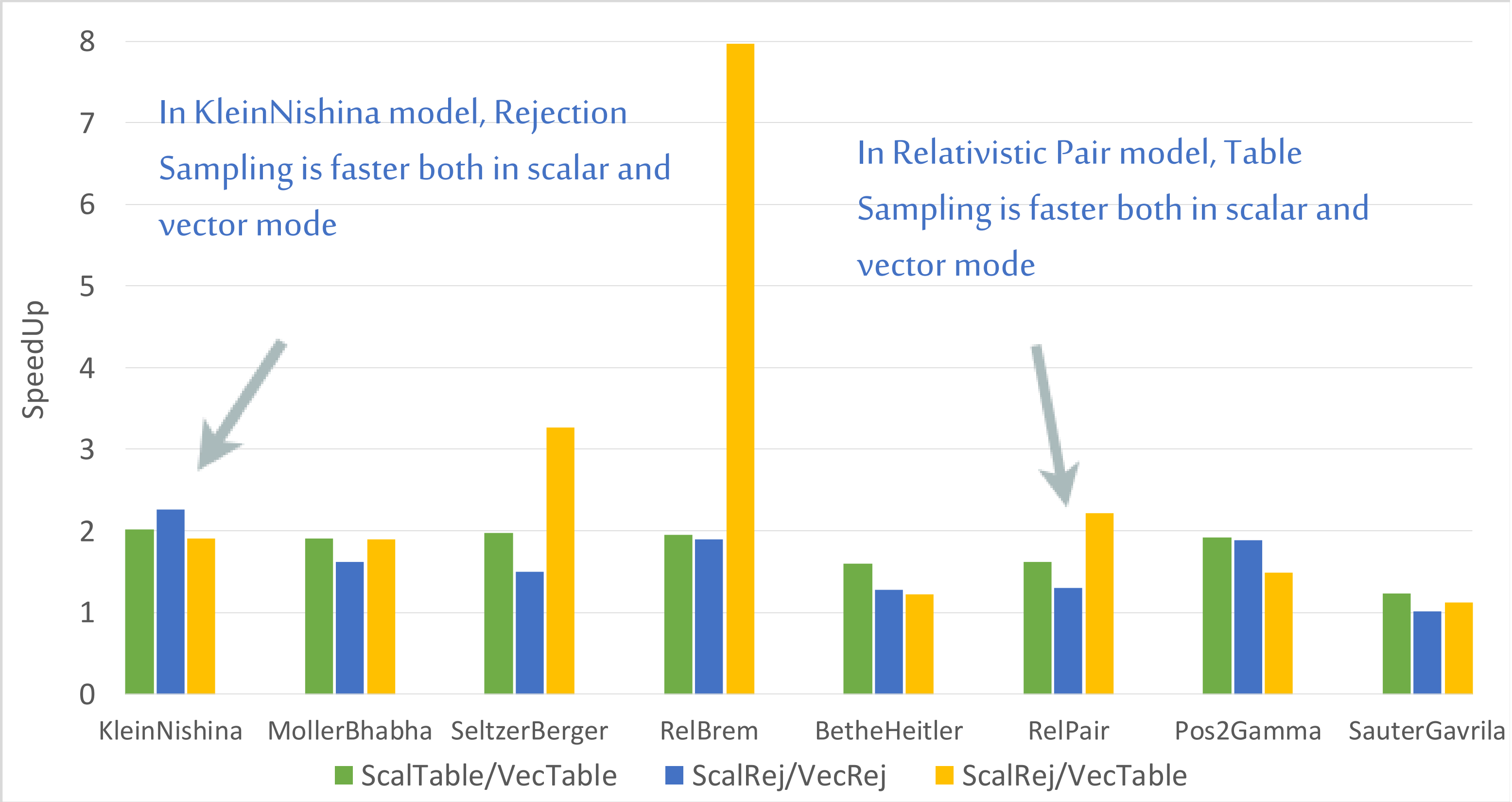
- Instruction Set: AVX2
- Backend: Vc
- Detector: Lead
- #baskets: 256
- Run with GoogleBenchmarks



M. Bandieramonte, M. Novak

Speedup from Vectorization of the **Table Sampling**

Speedup from vectorization of the **Rejection Sampling**

Speedup of **vectorized Table Sampling** w.r.t **scalar Rejection**

Speedup of the final state generation of different electromagnetic physics models obtained with SIMD vectorization in case of different sampling algorithms. The results were obtained by using Google Benchmarks on an Intel® Haswell Core™ i7-6700HQ, 2.6 GHz, with Vc backend and AVX2 instruction set processing 256 tracks.

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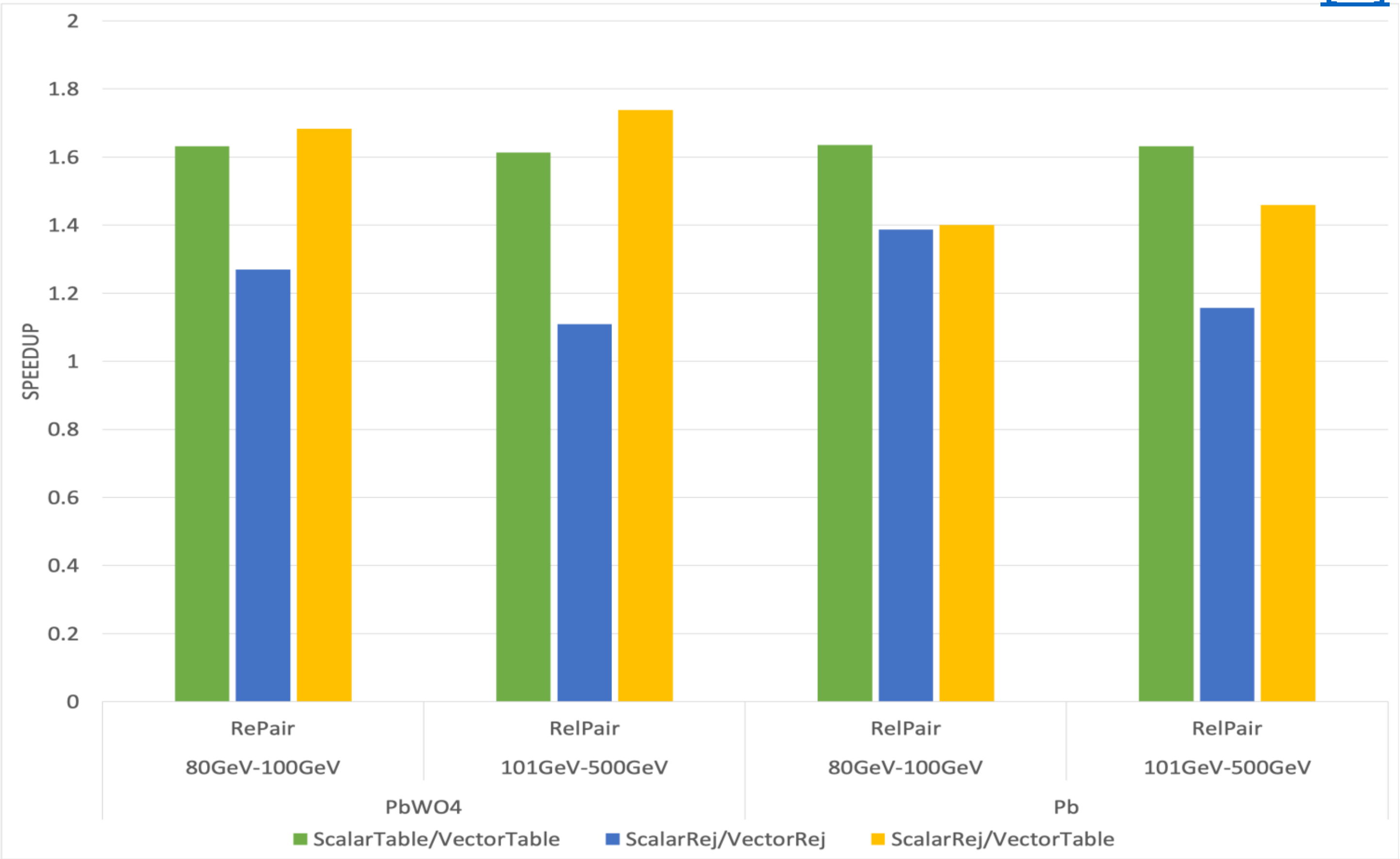

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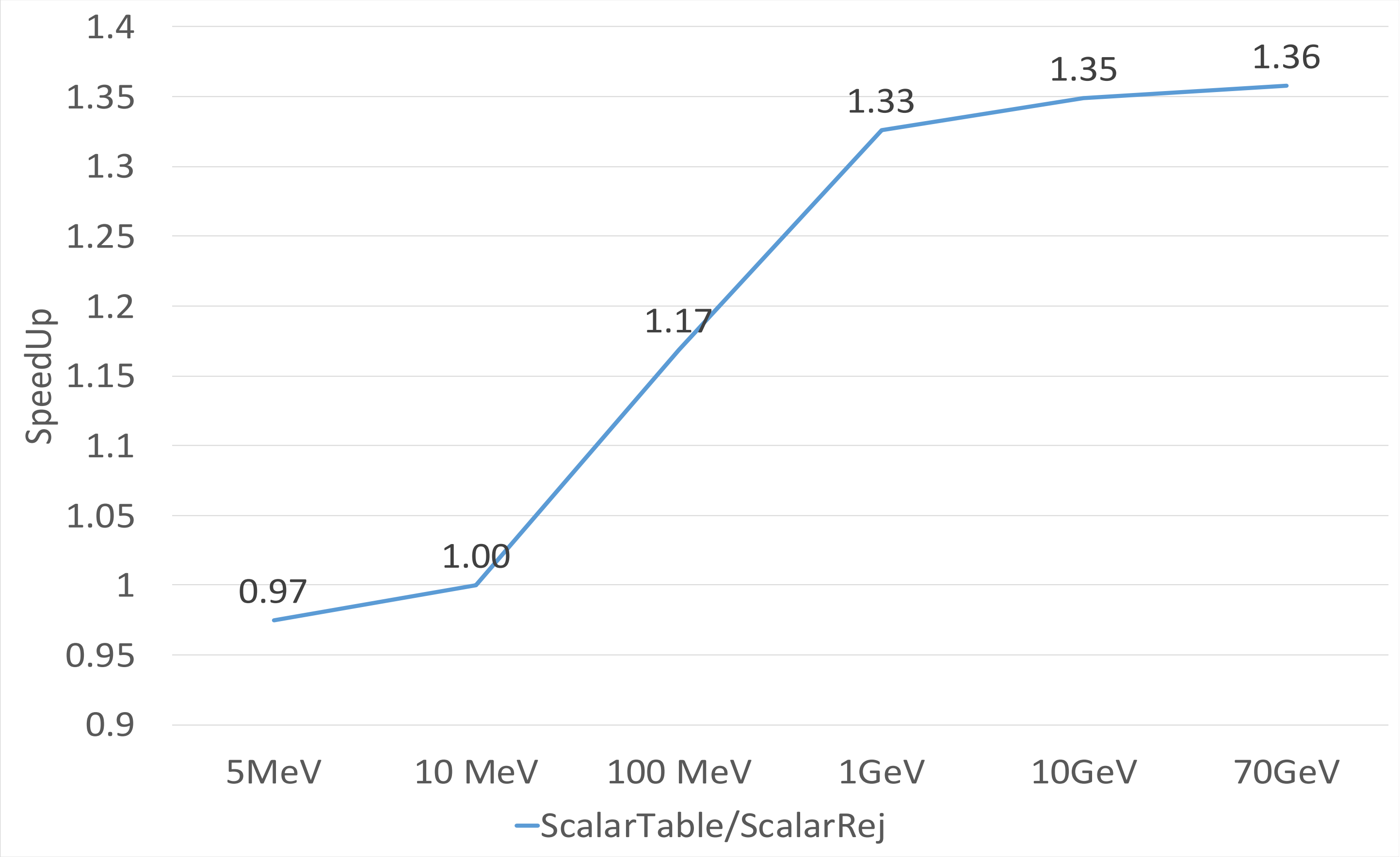

M. Bandieramonte, M. Novak

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Vectorized EM physics models – lesson learned

- Main message: there is **no generic solution** to achieve speedup
  - **Final state EM speedup**: between **1.5-3** on Haswell, **2-4** on Skylake with **AVX2**
  - **We never tested vectorized EM physics with AVX512 (speedup expected to be doubled): lack of person power**
- The **computational diversity** of the physics models directly implies a variation of the optimal algorithmic solution as a function of the models.
- In addition, the **dependence** of the underlying physics on some **external conditions** such as target material composition or primary particle energy introduces further variations
- In order to **maximize the achievable gain** from vectorization it's necessary to **profile** all the available final state generation algorithms as a function of:
  - The complexity of the underlying DCS
  - Target material composition
  - Primary particle energy
- **Due to lack of person power the profiling activity was not completed**

MC truth

Backup slides

GeantV kinematics output (MC truth)

- handling of MC truth is problematic per se
  - which particles to store, how to keep connections, where to connect hits
- multithreading adds the complexity
  - order of processing of particles is ‘random’
    - processing of ‘daughter’ particle may be completed before ‘mother’ particle ‘end of life’
  - events need to be ‘put together’ after parallel processing

MC truth

- we can’t (and we don’t need) to store all particles
  - typically no delta-e, no low-E gamma showers, etc needed
- we need to store particles necessary to understand the given event (process)
- we need to store particles to associate hits
- in all cases, we need to (re)connect particles to have consistent event trees

MC truth handling requirements

- no MC truth-handling strategy is perfect, nor complete, but:
  - we need to give user a way to decide
- transport need to provide/allow
  - links between mother and daughter particles
  - the possibility to flag particles as ‘to be stored’
  - possibility to introduce ‘rules’ what to store
  - a way to ‘reconnect’ tracks and hits if some are skipped
    - if we don’t store a particle, we need to update the daughter particles to point back to the last stored one in the chain
- for the final output we need to have some event record
  - for our proof of principle, we can start with HepMC

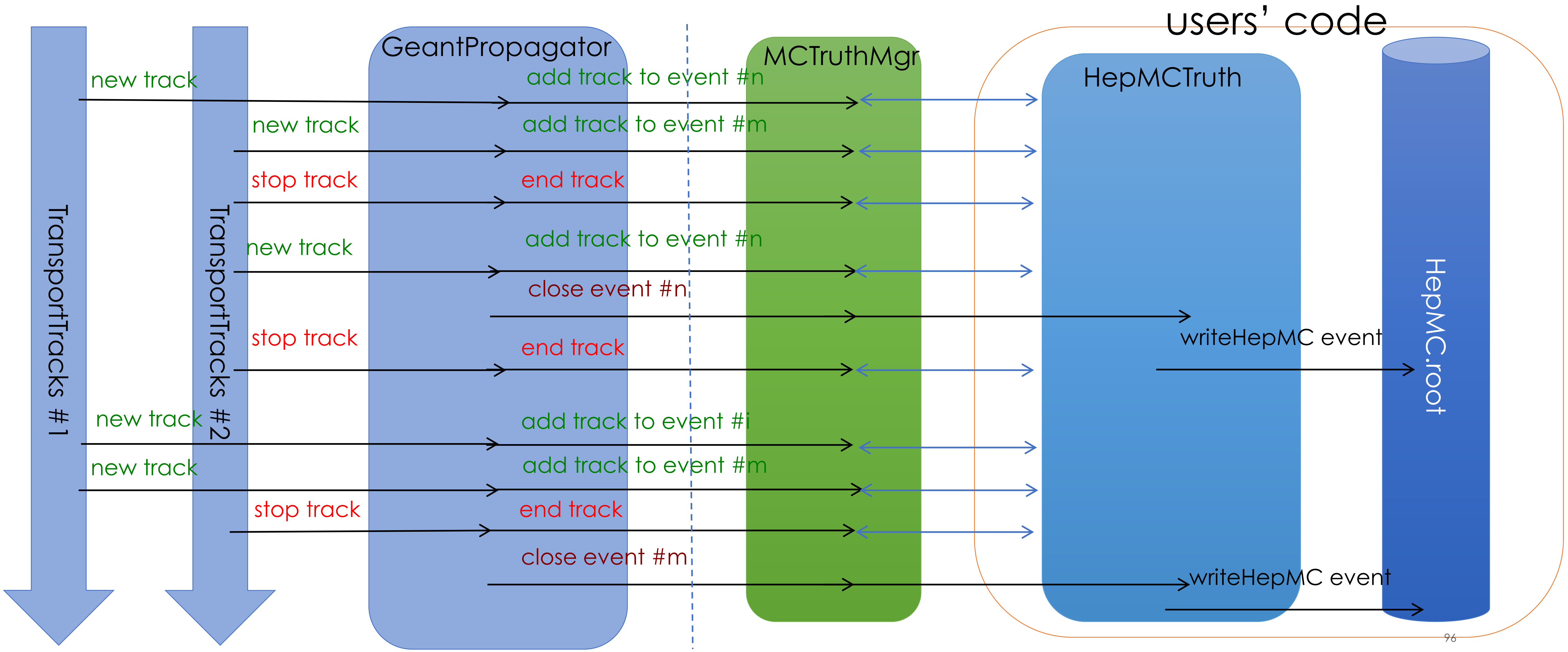
MC truth handling architecture

- light coupling to transport
  - minimal ‘disturbance’ to transport threads
  - maximal flexibility of implementing custom particle history handlers
- interface provided by MCTruthMgr
  - receives (concurrent) notifications from transport threads about
    - adding (primary or secondary) new particles
    - ending particles
    - finishing events
  - delegates processing of particles history to concrete MC truth implementation

MC truth infrastructure and users code

- MCTruthMgr provides interface and underlying infrastructure for particles history
  - light-weight transient, intermediate event record
- users code:
  - decision making (filtering) algorithm
  - conversion to users' event format
- concrete example implementation provided based on HepMC3

MC truth call sequence



MC truth output status

- GeantV MC truth manager provides handles to deal with particles history
  - allows ‘physics’ studies
  - first implementation, further iterations possible to look in detail at performance
- example implementation based on HepMC3 provided
- further performance testing/improvements in highly concurrent environment to be studied

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Backup slides

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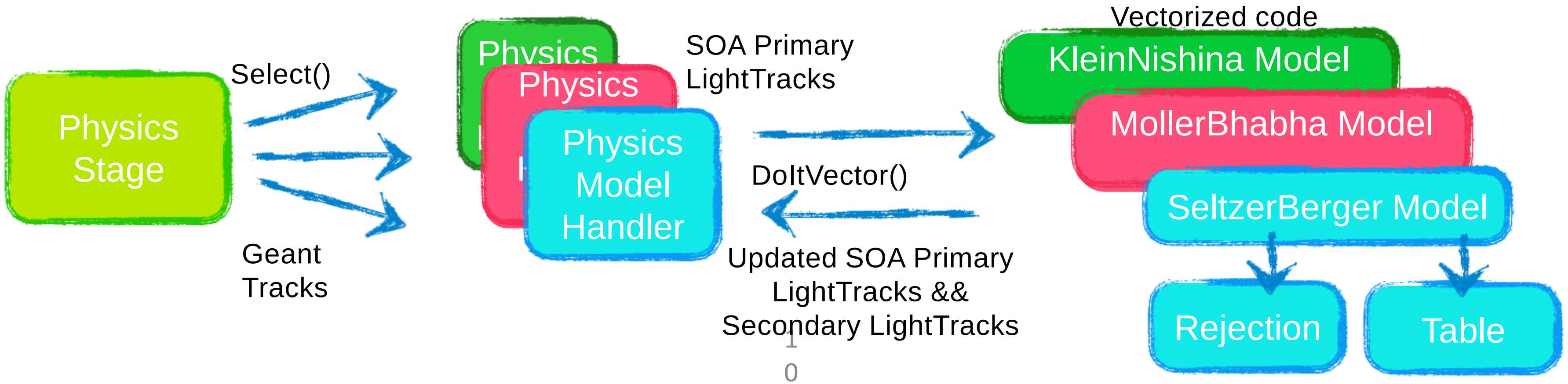

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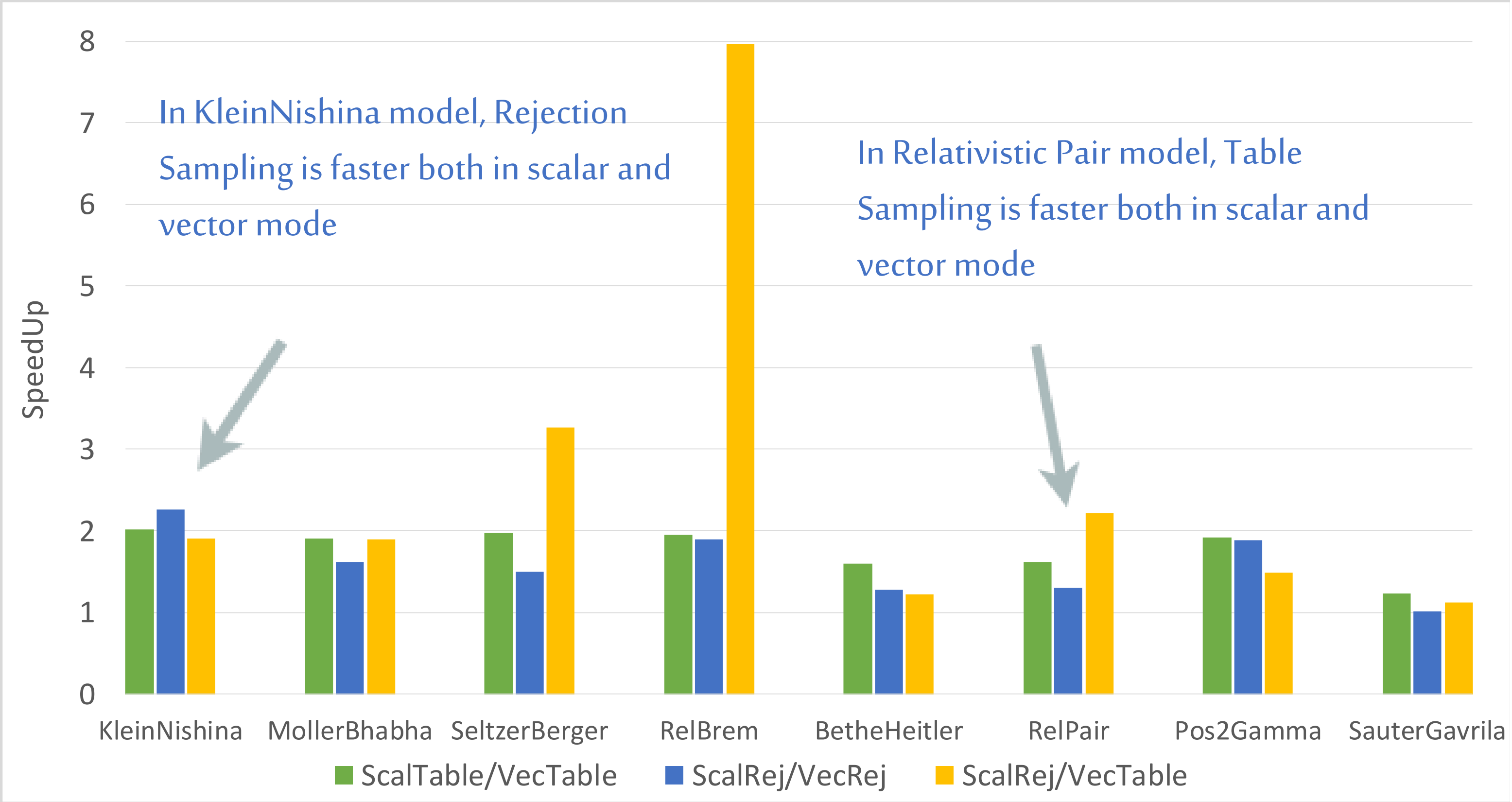

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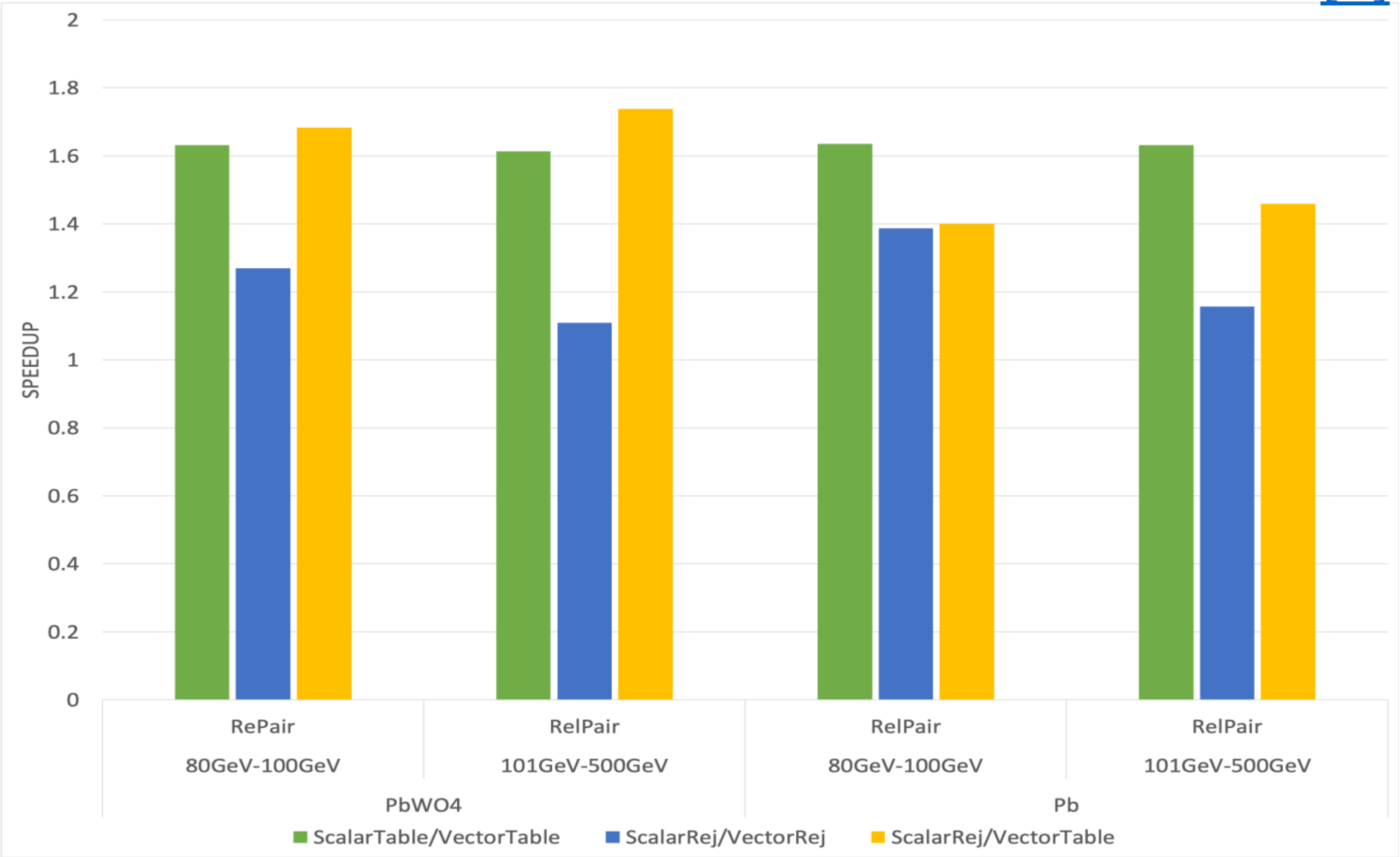

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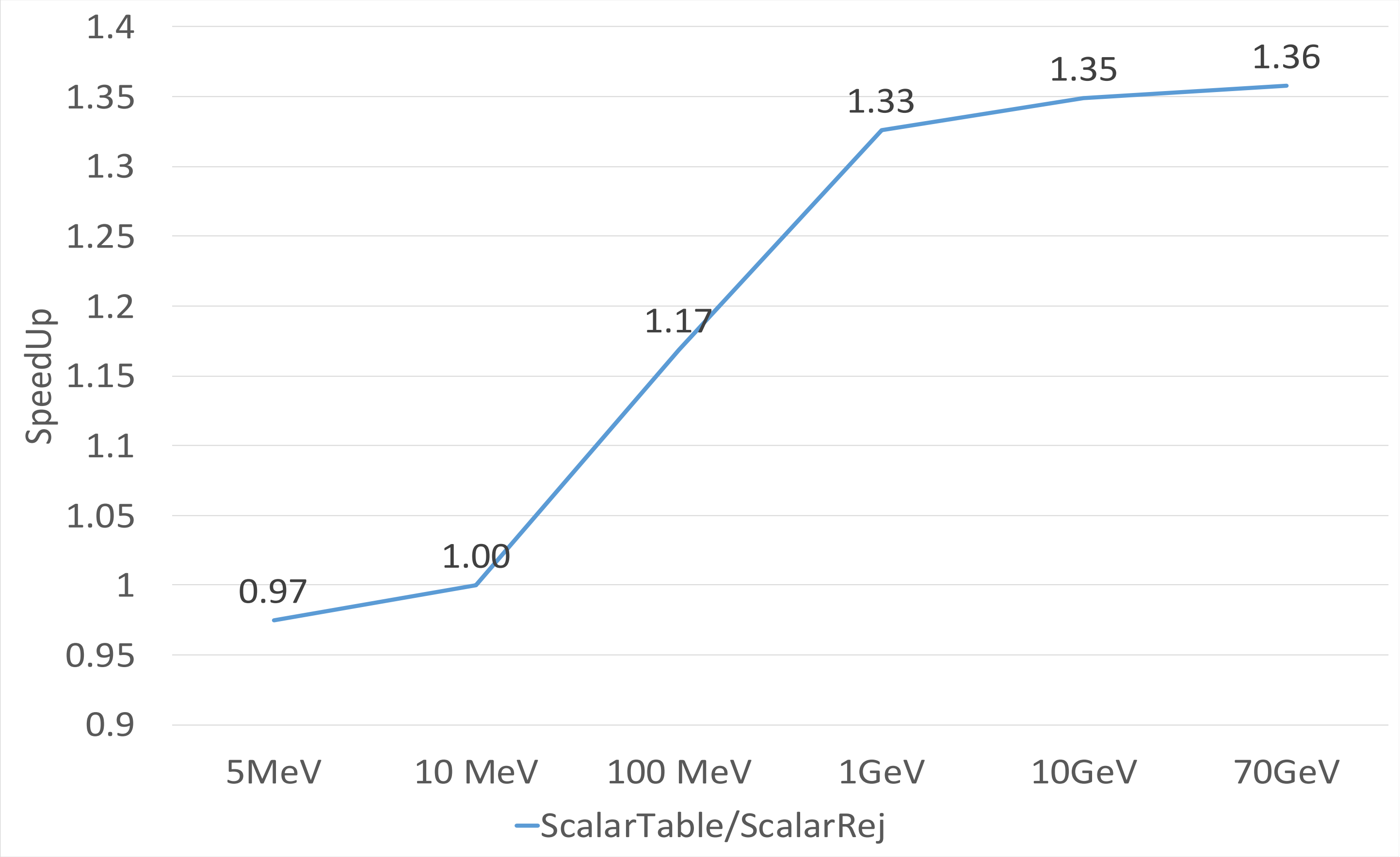

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5. Performance results

Backup slides

Performance Comparisons: Tested Platforms

- Process-Cores-CPU[GHz]-Memory[GB]-Cache[MB]-SIMD

Processor	Core	CPU	Mem	Cache	SIMD
Intel E2620 (Sandy Bridge)	2x6	2.0	32	15	AVX
Intel E2680 (Broadwell)	2x14	2.4	128	35	AVX2
AMD 6128 (Opteron)	4x8	2.3	64	15	SSE4

- Cache size

Processor(*)	L1 set	L2 set	L3 set
AVX-2.0-15	6x32 KB 8-way	6x256 KB 8-way	15 MB 20-way
AVX2-2.4-35	4x32 KB 8-way	14x256 KB 8-way	35 MB 20-way
SSE4-2.3-15	8x64 KB 2-way	8x 512 KB 16-way	2x6 MB

  - * Processor Convention: SIMD-CPU-Cache

Locality

- Single track mode (strk)
  - Emulate Geant4 style tracking
  - A meaure of locality: GeantV (strk)/GeantV(default)
- CPU Time in [sec] and their ratios

Processor	GeantV	GeantV-strk	strk/default
AVX-2.0-15	2621	2960	1.13
AVX2-2.4-35	1628	1533	0.94
SSE4-2.3-15	4457	4817	1.08

  - The data locality does not explain the performance difference between Geant4 and GeantV (scalar)

Hardware Counters: L2 Cache and L3 Cache

- L2 cache miss (~12 cycles): in [Billion] counters

Processor	GV (ICM)	G4(ICM)	GV (DCM)	G4(DCM)
AVX-2.0-15	20	36	89	46
AVX2-2.4-35	24	37	100	51
SSE4-2.3-15	16	3.3	55	8.9

  - ICM (DCM) = Instruction (data) cache miss
  - GeantV has less ICM and Geant4 has less DCM (AVX/AVX2)

- L3 cache miss (~38 cycles): in [1B] counters

Processor	GV (TCM)	G4(TCM)	GV (TCA)	G4(TCA)
AVX-2.0-15	1.9	0.19	109	80
AVX2-2.4-35	1.3	0.012	126	82
SSE4-2.3-15	N/A	N/A	N/A	N/A

  - TCM (TCA): Total Cache Miss (Access)

Performance summary table (go to backup)

Normalized performance factor with respect to the Intel i7 2.5GHz taking into account the clock speed

CPU	OS	gcc	SIMD	Cache	GV	G4 [sec]
Intel i7 2.5GHz	Ubuntu 16.04	5.4.0	AVX2	8 MB	1 ± 0.01	1 ± 0.03
Intel Core i7-4510U 2GHz	Ubuntu 16.04	5.4.0	AVX	4MB	1.39 ± 0.01	0.98 ± 0.01
AMD A10-7700k	Fedora Workstation 29	8.2.1	AVX	4 MB	1.94 ± 0.01	2.48 ± 0.02
Intel R 1.8GHz	Fedora Workstation 29	8.3.1	SSE4	2 MB	2.95 ± 0.01	2.15 ± 0.01
Intel Centrino 2	Fedora Workstation 29	8.2.1	AVX±	4 MB	2,76 ± 0.01	3.75 ± 0.02
11AMD e-300	Ubuntu 18.10	8.2.0	SSE2	1 MB	Not Vc compatible	13.32 ± 0.01

Geant4 fluctuates more than GeantV over different tested platforms

Integration with experimental frameworks

Backup slides

Status of GeantV Integration in CMSSW

Kevin Pedro, Sunanda Banerjee

(FNAL)

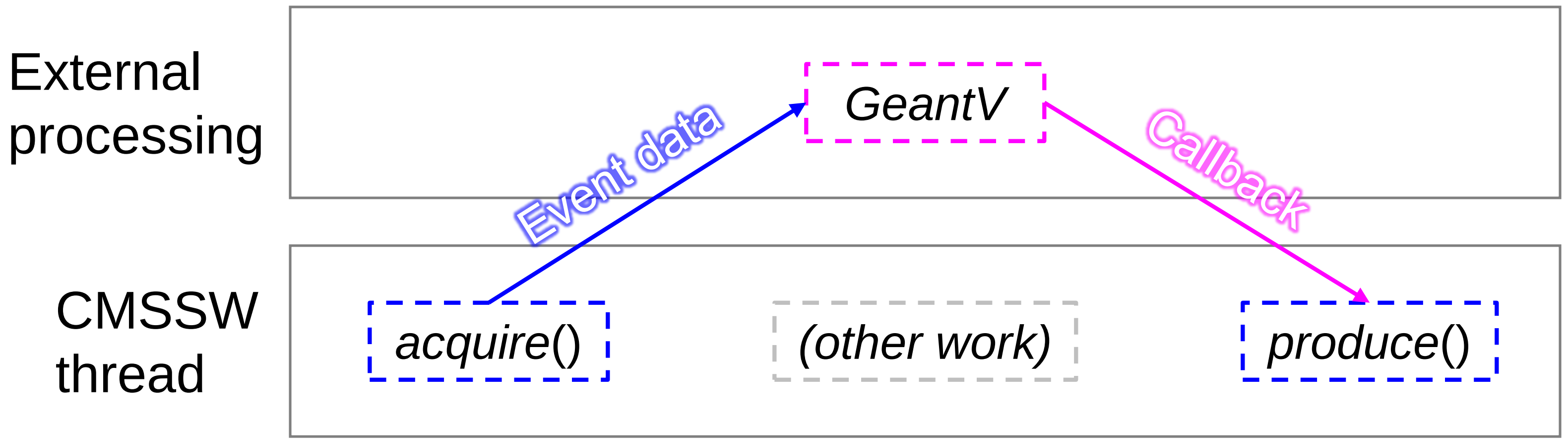
October 4, 2019

Introduction

- Integration testing of GeantV w/ CMSSW has several goals:
  - Demonstrate benefits of co-development between R&D team & experiments
  - Exercise capabilities of CMSSW framework to interface with external processing (ExternalWork mechanism) and handle track-level parallelization in detector simulation
  - Measure any potential CPU penalties when running GeantV in CMSSW
  - Estimate cost of adapting to new interfaces and eventually migrating to new (and potentially backward-incompatible) tools such as GeantV
    - Thinking forward to HPC/GPU solutions
- *Not* planning to migrate CMS simulation to GeantV
  - This is an R&D exercise

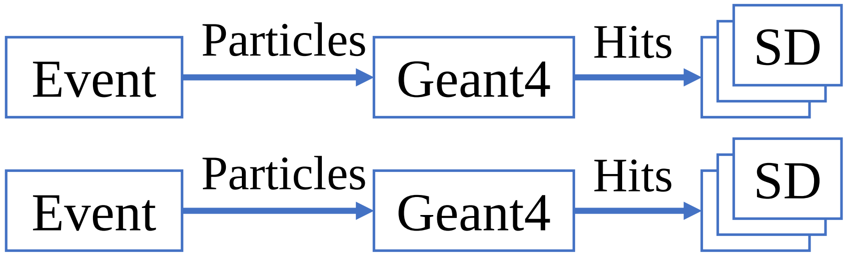
GeantV Integration Tests in CMSSW

- Repositories: install-geant, SimGVCore
- ✓ Generate events in CMSSW framework, convert HepMC to GeantV format
- ✓ Build CMSSW geometry natively and pass to GeantV engine (using TGeo)
- Using constant magnetic field, limited EM-only physics list
- ✓ Calorimeter scoring adapted
- ✓ Run GeantV using CMSSW ExternalWork feature:
  - Asynchronous, non-blocking, task-based processing
- ✓ Output in CMS format, immediately suitable for digitization etc.

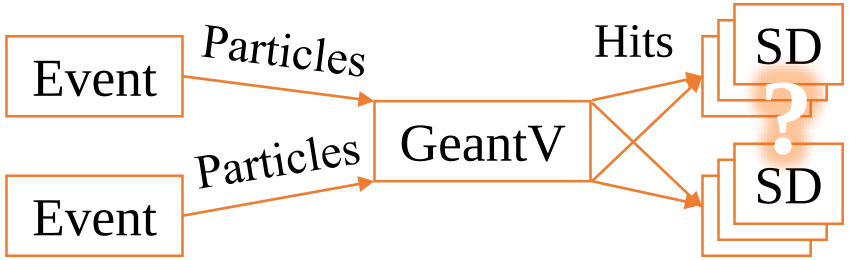


Geant4 vs. GeantV Scoring

- Sensitive detectors (SD) and scoring trickiest to adapt
  - Necessary to test "full chain" (simulation → digitization → reconstruction)
  - Significantly more complicated than Geant4 MT



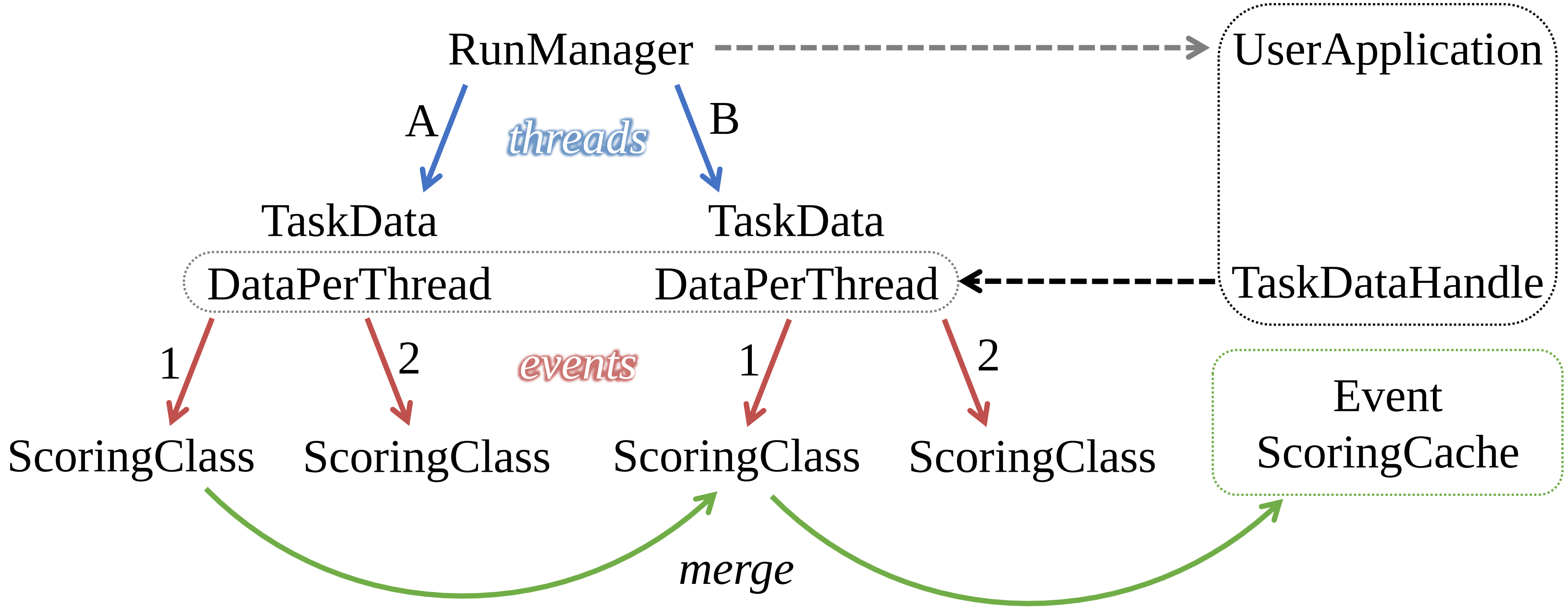
Geant4 shares memory, but each event processed in separate thread



Each event processed in multiple threads, mixed in with other events

- Duplicate SD objects per event per thread, then aggregate → 4 streams, 4 threads = 16 SD objects
  - GeantV TaskData supports this approach
- ➢ Use template wrappers to unify interfaces and operations
  - Ensure exact same SD code used for Geant4 & GeantV
  - Minimize overhead (no branching or virtual table)

GeantV Data Aggregation



- Each ScoringClass object has instance of CaloSteppingAction
  - Some additional memory overhead from duplicated class members
    - Attempt to minimize this by storing volume maps in magic static struct
- Merged ScoringClass output copied to cache attached to Event object
  - GeantV may consider event finished before CMSSW has written output → copy to cache, then immediately clear ScoringClass objects (avoid possible race conditions)

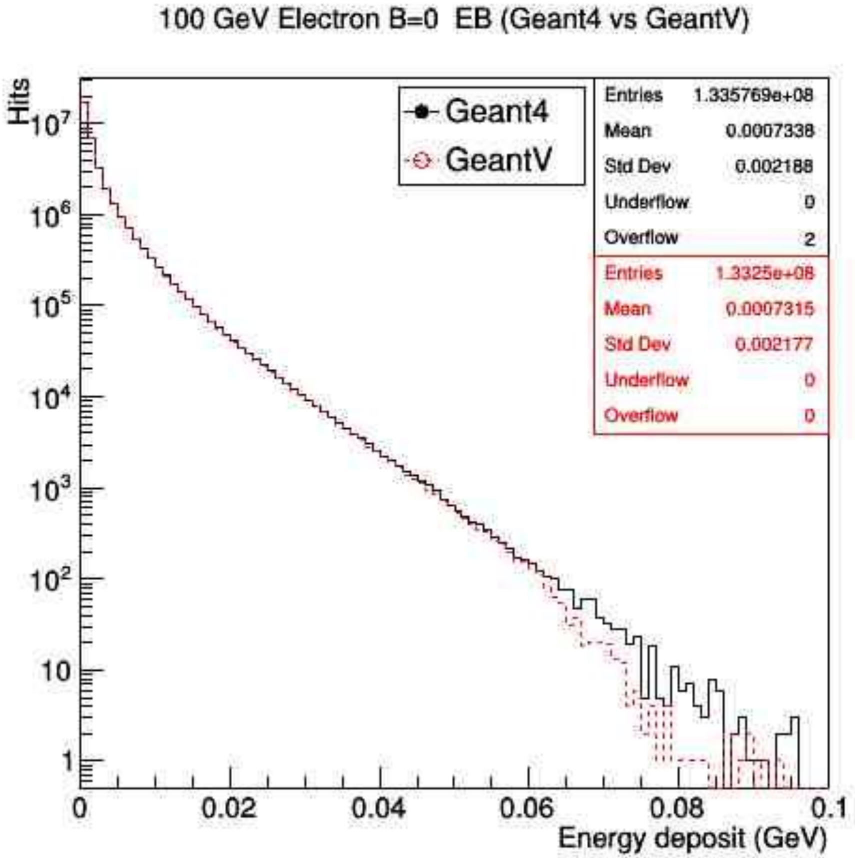
Physics Validation

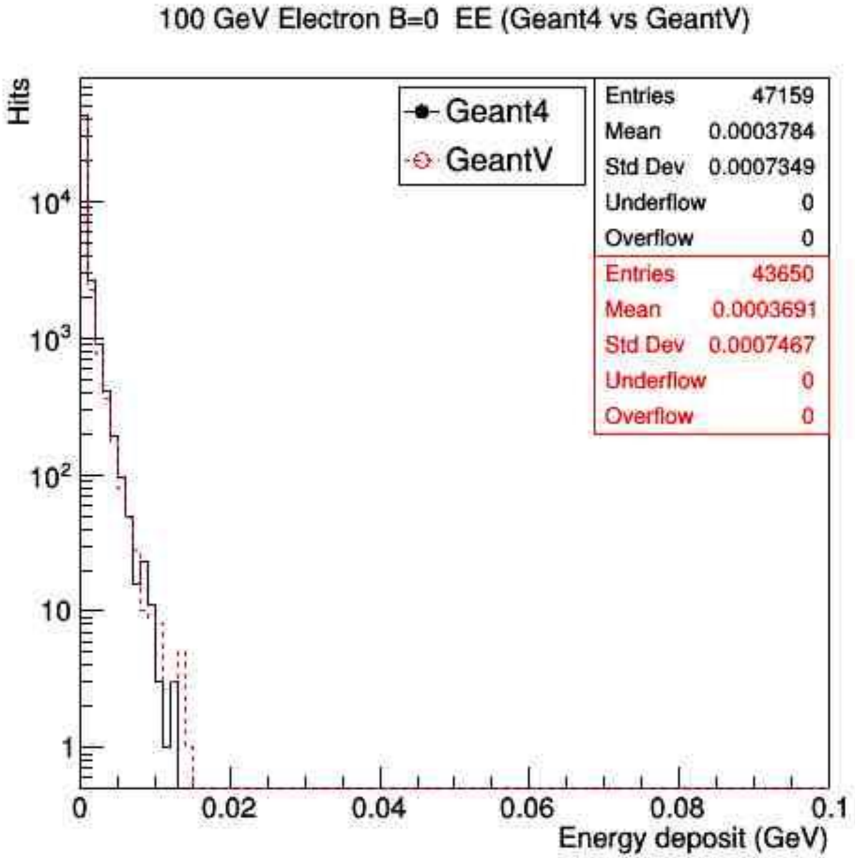
- Settings:
  - Geant4 10.4p2 w/ VecGeom v0.5 (scalar)
  - GeantV pre-beta-7 w/ VecGeom v1.1
  - All CMS-specific G4 optimizations disabled
  - Same production cuts (default 1mm)
  - Single thread (reproducible pRNG sequences)
  - Generate 1000 events w/ single electron, $E = 100$ GeV, $\eta = 1.0$, $\varphi = 1.1$
- Tests: (same generated events used for G4 and GV)

1. No field ($B = 0$)
2. Constant field ($B = 3.8$ T)

(more in backup)

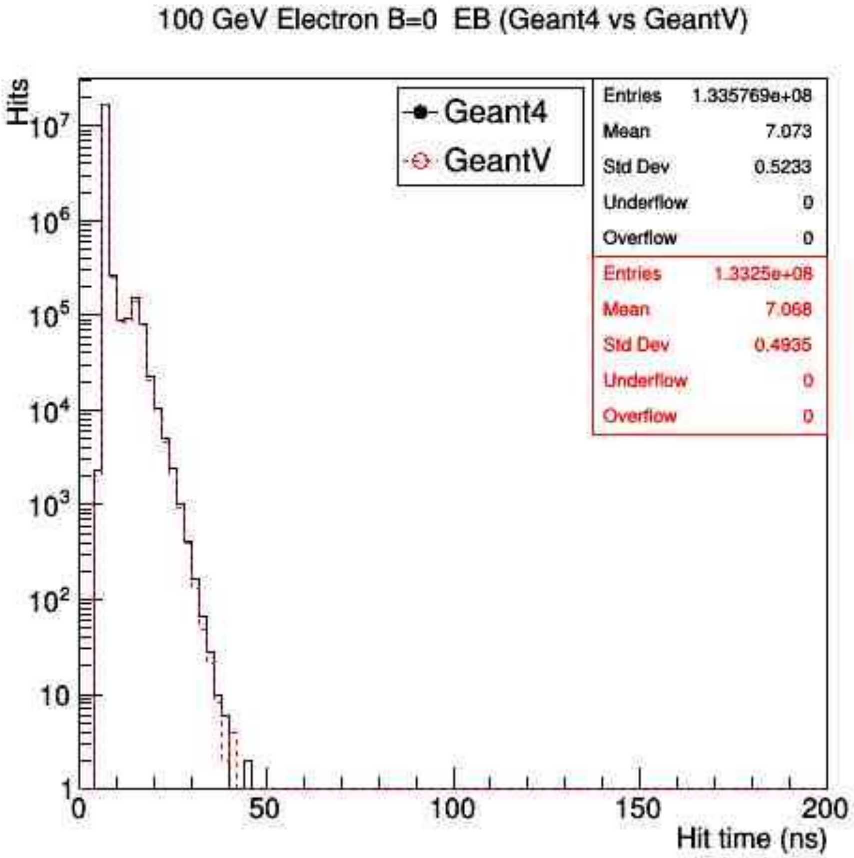
1. Energy Deposits for 100 GeV e- (B=0)

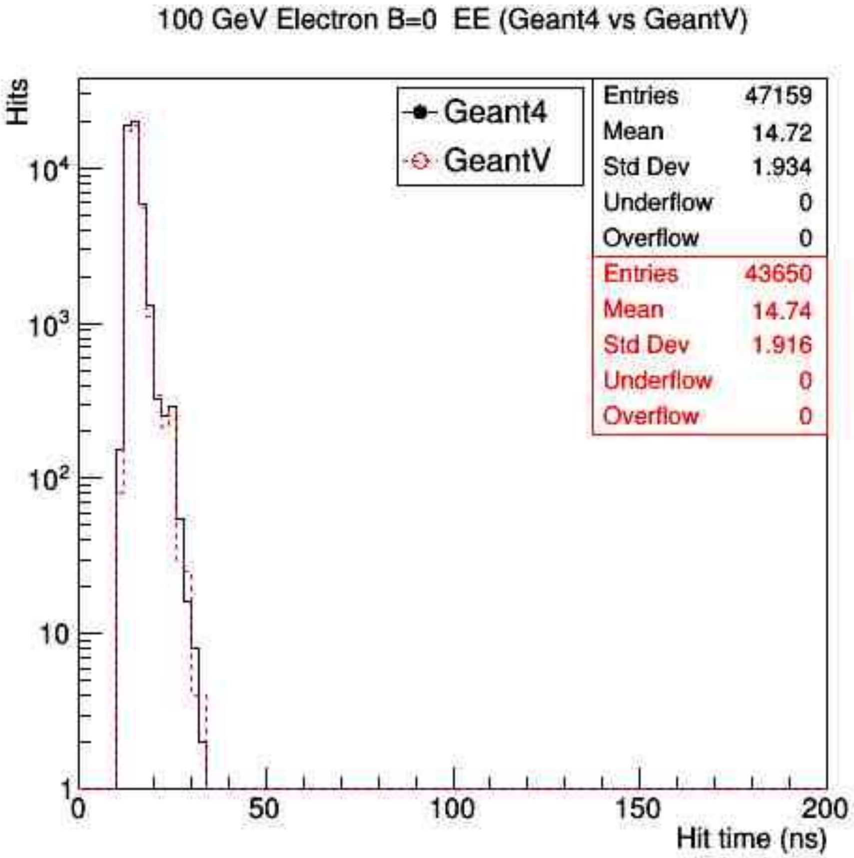




- The number of entries differs by 0.3% (7.4%) in EB (EE)
- The means differ by 0.2% for EB and 2.5% for EE

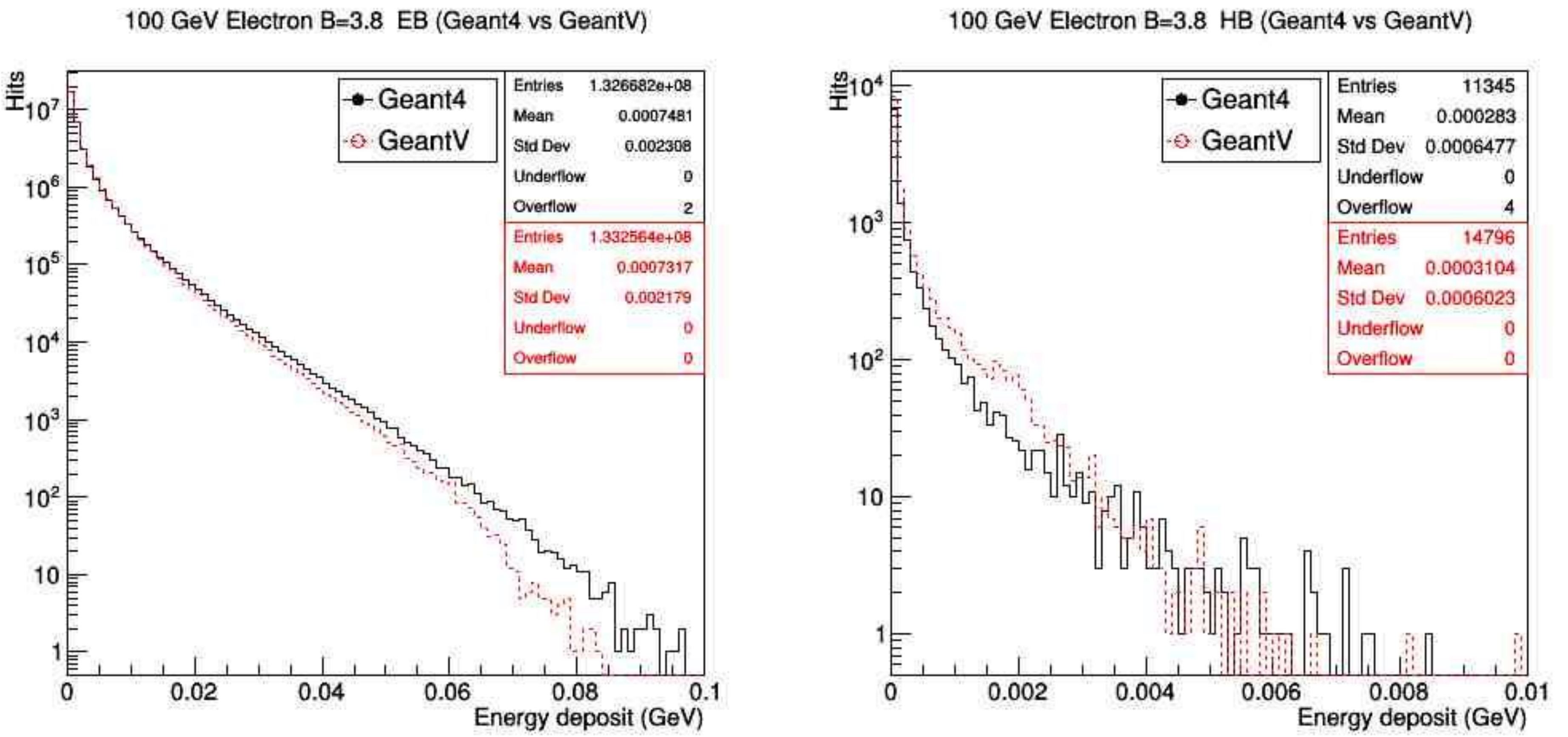
1. Hit Time for 100 GeV e- (B=0)





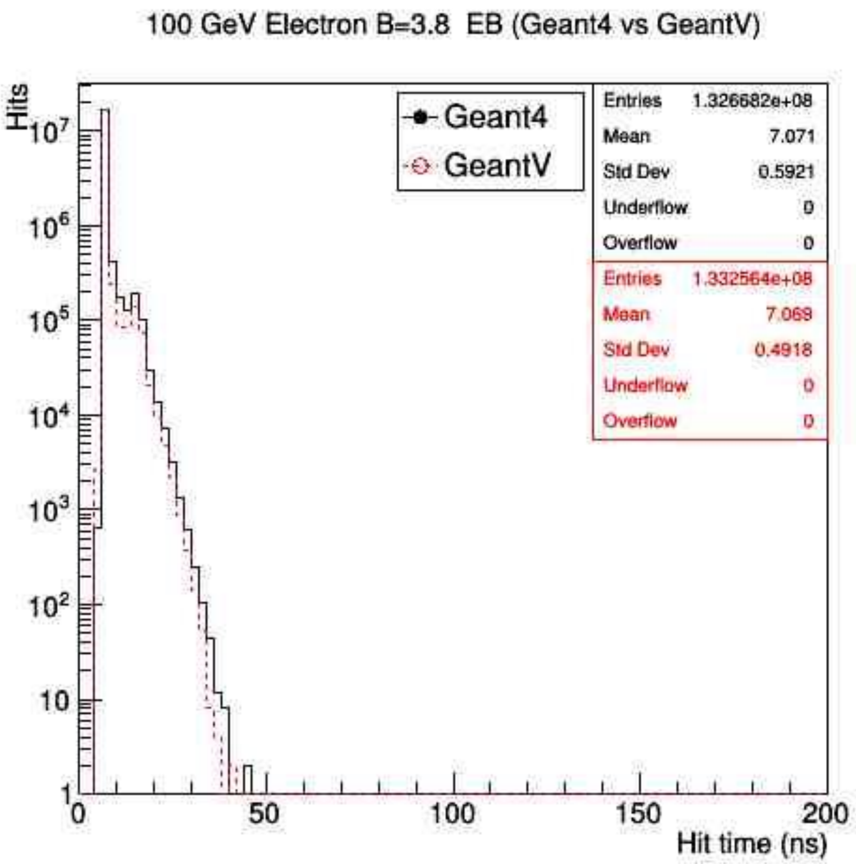
- Means differ by 0.07% for EB and 0.13% for EE
- GeantV and Geant4 applications provide roughly the same distributions

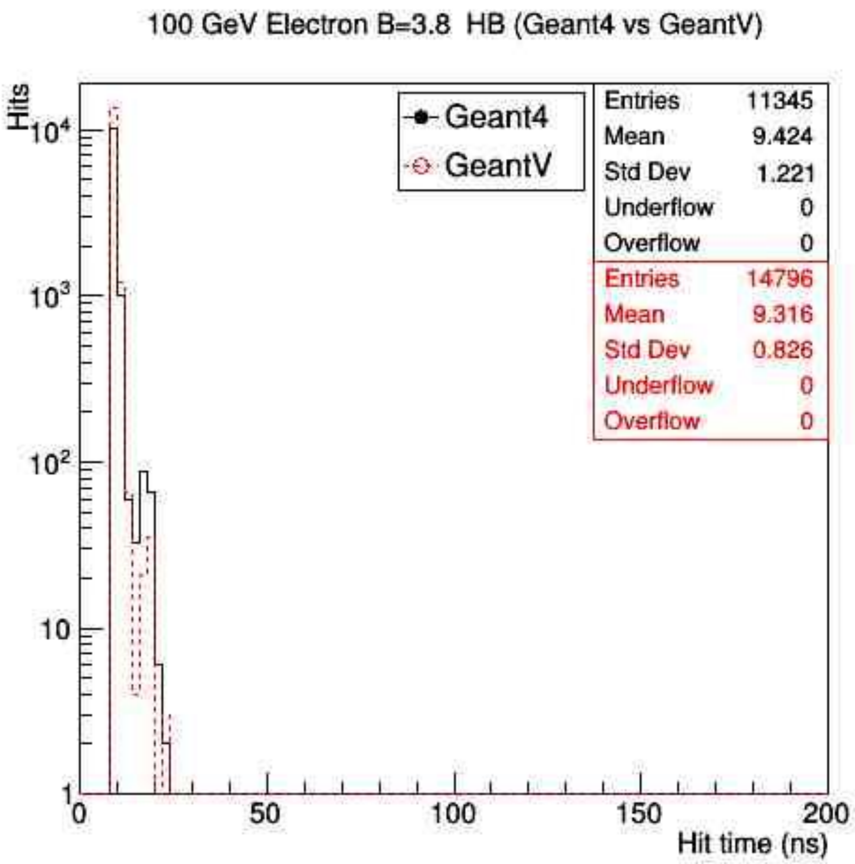
2. Energy Deposits for 100 GeV e- (B=3.8)



- The number of entries differ by 0.4% (23.3%) in EB (HB)
- The means differ by 2.2% for EB and 8.8% for HB

2. Hit Time for 100 GeV e- (B=3.8)





- The means differ by 0.03% for EB and 1.15% for HB
- There is a small difference in the physics results of GeantV and Geant4 applications in the presence of B-field

Performance Tests

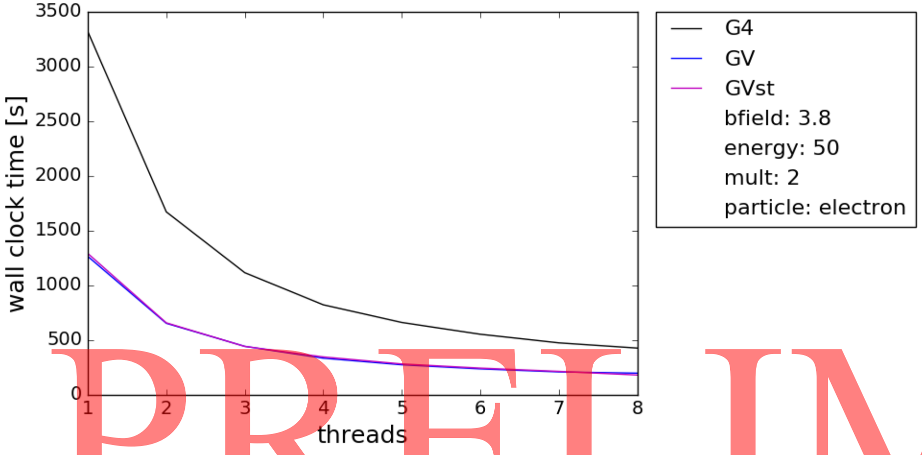
- Settings:
  - GeantV pre-beta-7+ (63468c9b)
    - Enabled: vectorized multiple scattering, field (not physics)
  - Generate 500 events, 2 electrons w/ E = 50 GeV, random directions
  - Keep # events / thread constant (copy & concat 500 generated events)
  - Use same generated events in G4 and GV
  - Keep unused threads busy
  - Disable output
- Machine: FermiCloud VM w/
  - Intel(R) Xeon(R) CPU E5-2660 v2 @ 2.20GHz, 4096 KB cache
  - sse4.2 instructions
- Track wall clock time & memory with CMSSW TimeMemoryInfo tool
  - Measures VSIZE, RSS per event
  - Calculate speedup from wall time
    (divided by # threads used, since # events / thread is constant)

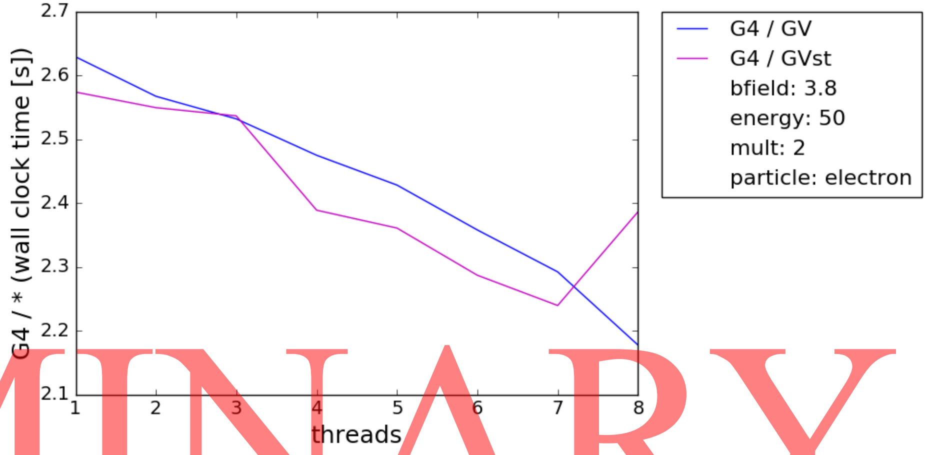
Characterization

- VM CPU has relatively small cache
  - Known that major component of GeantV speedup arises from smaller library → fewer cache misses
- To characterize CMSSW performance results, first run built-in GeantV FullCMS standalone test
  - Single thread, settings as close to previous slide as possible (see test script: testStandalone.sh)
  - NB: different physics list used in standalone vs. CMSSW
- Results:
  - GeantV: RealTime=756.002s CpuTime=753.09s
  - Geant4: User=1617.36s Real=1618.52s

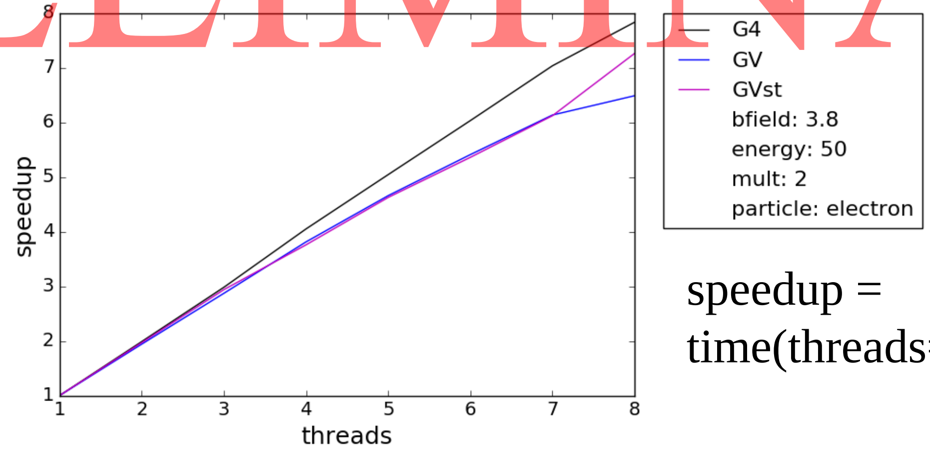
→2.14× speedup (standalone)

Time Performance





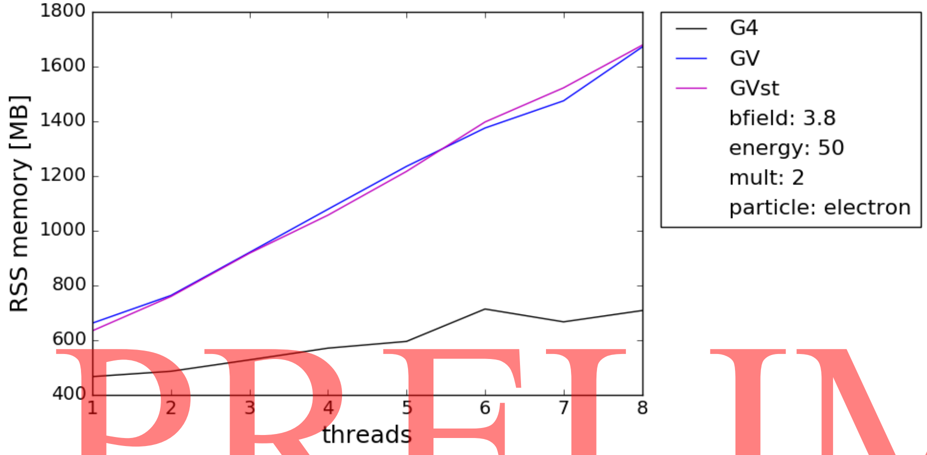
PRELIMINARY

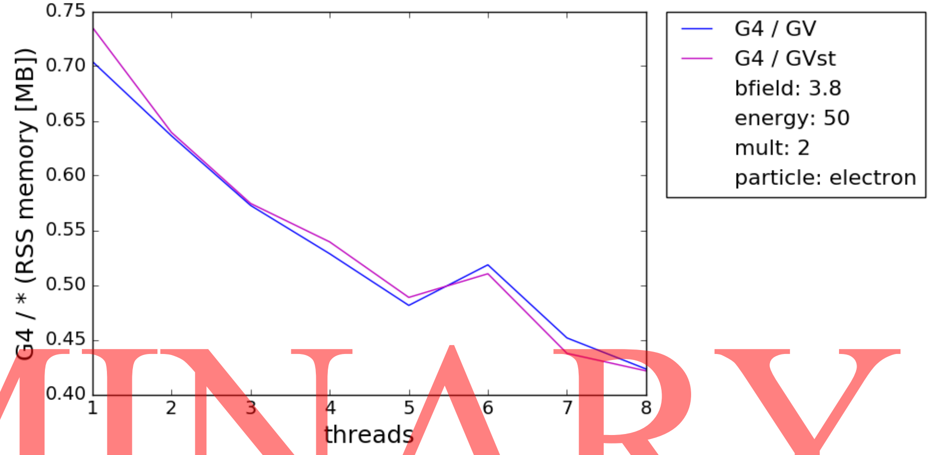


speedup = time(threads=1)/time(threads=N)

- GV 2.6× faster than G4 single thread, still ~2.2× faster in MT
- GV single track mode similar to basketized
- G4 has better scaling w/ # threads than GV

Memory Performance





PRELIMINARY

- Memory grows ~linearly w/ # threads (expected)
- GV uses more memory than G4 (expected)
- Single track mode uses similar memory to basketized

What Would Be Next?

- To complete the goals of CMS R&D studies for the paper:
  - Full magnetic field map
  - Test on machines w/ different cache sizes
- Stretch goals/notes for future similar projects:
  - Random number generator
  - Adapt scoring classes for other detectors (beyond calorimeters)
  - Combine w/ other simulation improvements
    - Notably Russian Roulette & HF shower library, which give largest gains
- If GeantV project were to continue:
  - Better solution for geometry conversion than TGeo
  - Sensitive volume/detector functionality
  - Vectorized hadronic physics
  - Improve threading, memory management, and ownership models
  - Decouple event loading & task launching in ExternalLoop mode
  - Event-wise scoring rather than current thread-wise scoring w/ TaskData

Conclusions

- CMS studies met ~all goals laid out
  - Co-development led to improvements and bug fixes in GeantV to facilitate experiments' use
  - One of the first projects to exercise CMSSW ExternalWork feature
  - Physics validation & CPU measurements show very positive results
  - Path to adapt interfaces efficiently is laid out:
    "Rosetta stone" mostly contained in StepWrapper and VolumeWrapper

Geant4	GeantV
StepWrapper	StepWrapper
VolumeWrapper	VolumeWrapper

- Demonstrator to test major elements of GeantV-CMSSW integration is ready
  - Up to 2.6× speedup in CMSSW application
  - Will finalize results for paper
  - The CMS simulation group thanks the GeantV R&D team for providing support to this integration exercise and making it a successful co-development endeavor

Extras

Template Wrappers

- **Goal**: use *exact same* SD code for Geant4 and GeantV
- Problem: totally incompatible APIs
  - Example: `G4Step::GetTotalEnergyDeposit()` vs. `geant::Track::Edep()`
- Solution: template wrapper with unified interface
  e.g. `StepWrapper<T>::getEnergyDeposit()`
  - SD code *only calls* the wrapper
  - Wrapper stores pointer to T (minimize overhead)
- Current wrappers:
  - BeginRun
  - BeginEvent
  - Step
  - Volume
  - EndEvent
  - EndRun

Traits

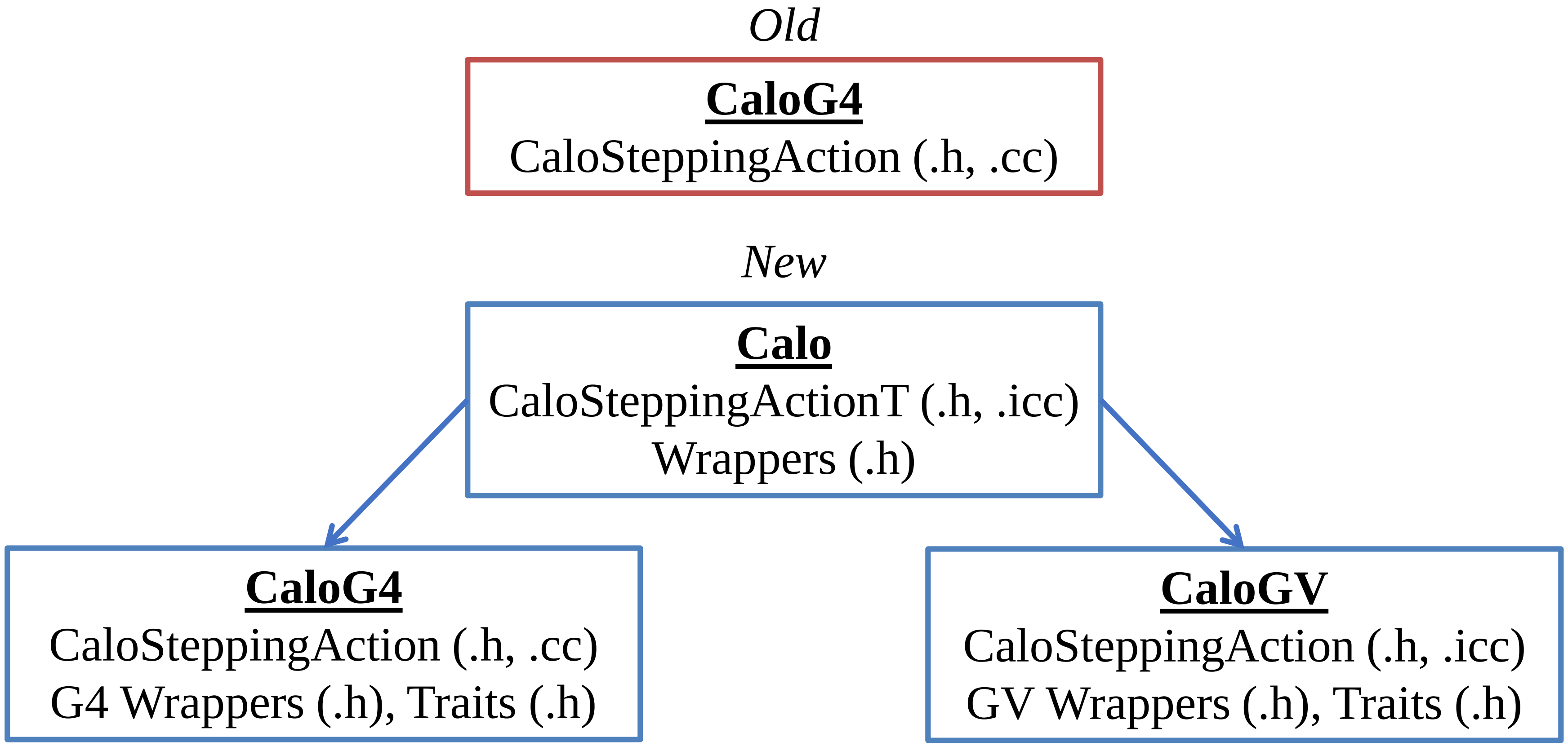
- Collect Geant4/GeantV-specific types and wrappers into unified **Traits** class:

```
struct G4Traits {
  typedef G4Step Step;
  typedef sim::StepWrapper<Step> StepWrapper;
};
struct GVTraits {
  typedef geant::Track Step;
  typedef sim::StepWrapper<Step> StepWrapper;
};
```

- Provides standardized typenames to be used by SD class:

```
template <class Traits> class CaloSteppingActionT : …,
  public Observer<const typename Traits::Step *>
{
  public:
    void update(const Step * step) override {
update(StepWrapper(step)); }
  private:
    // subordinate functions with unified interfaces
    void update(const StepWrapper& step);
};
```

Organization



- SD interface & implementation in **Calo** (.icc file), w/ unimplemented wrapper interfaces
- G4/GV wrapper specializations in **CaloG4/GV**, w/ specific instances of templated SD class → isolate dependencies

Scoring Approaches

- Two approaches to scoring in CMSSW:

1. Inherit from **G4VSensitiveDetector** (Geant4 class)
   → automatically initialized for geometry volumes marked as sensitive
2. Inherit from **SimWatcher** (CMSSW standalone class)
   → need to specify names of watched geometry volumes

- CaloSteppingAction is a demonstrator class w/ approach 2
  - Simplified version of ECAL and HCAL scoring
  - Less dependent on Geant4 interfaces
- "Real" SD code uses approach 1

➢ More work to extract Geant4 dependencies will be necessary
  - Some SD class methods directly from Geant4 (via inheritance)
  - Need to mock up Geant4-esque interfaces w/ dummy classes for GeantV

More Physics Validation

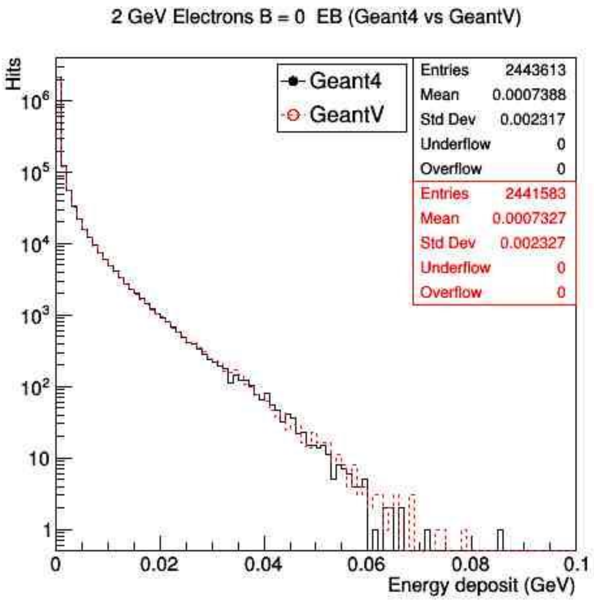
3. Generate 1000 events of single electrons at 2, 10 and 50 GeV at a fixed direction and compare GeantV against Geant4 with magnetic field off and on at 3.8 Tesla

4. Generate 100 events of 50 GeV double electrons at 50 GeV with $-3 < \eta < 3$ and $0 < \varphi < 2\pi$, run in multi-threaded mode (4 threads), B = 0 Tesla

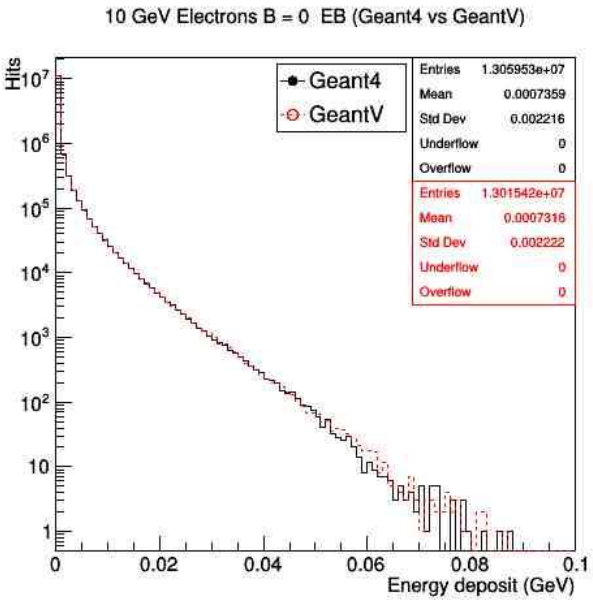
5. Repeat multi-threaded test with B = 3.8 Tesla

3. Energy Deposit with B = 0

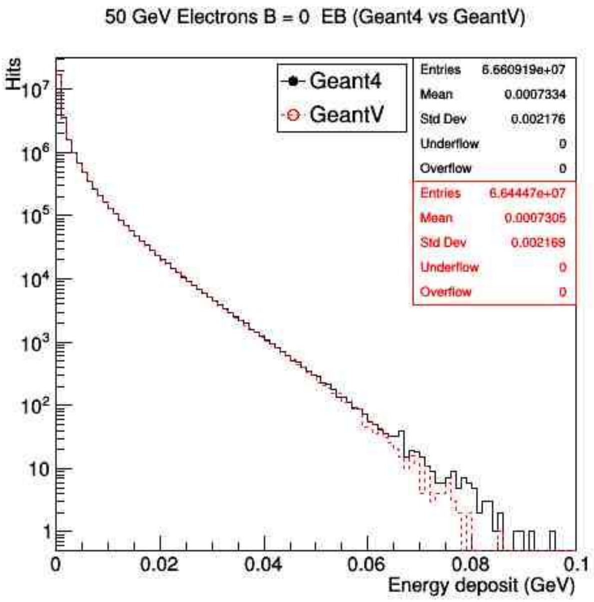
2 GeV Electrons



10 GeV Electrons



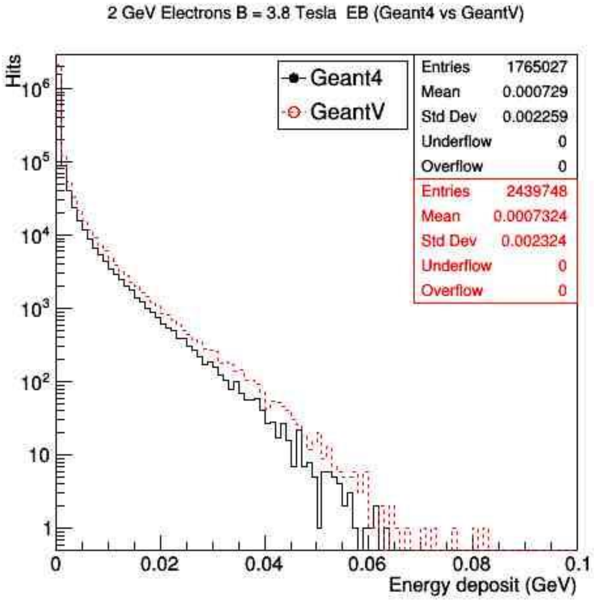
50 GeV Electrons



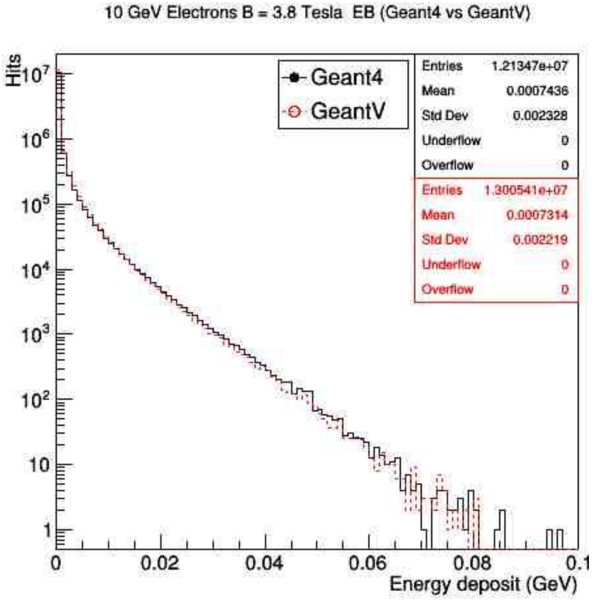
- Number of hits is the same for all 3 energies. The differences are at the level of 0.1/0.3/0.2% for 2, 10 and 50 GeV
- The means differ by 0.8/0.6/0.4% at the three energies

3. Energy Deposit with B = 3.8

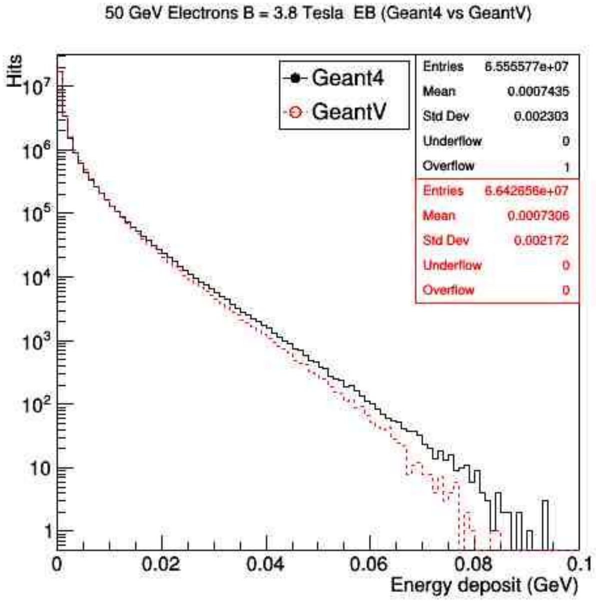
2 GeV Electrons



10 GeV Electrons

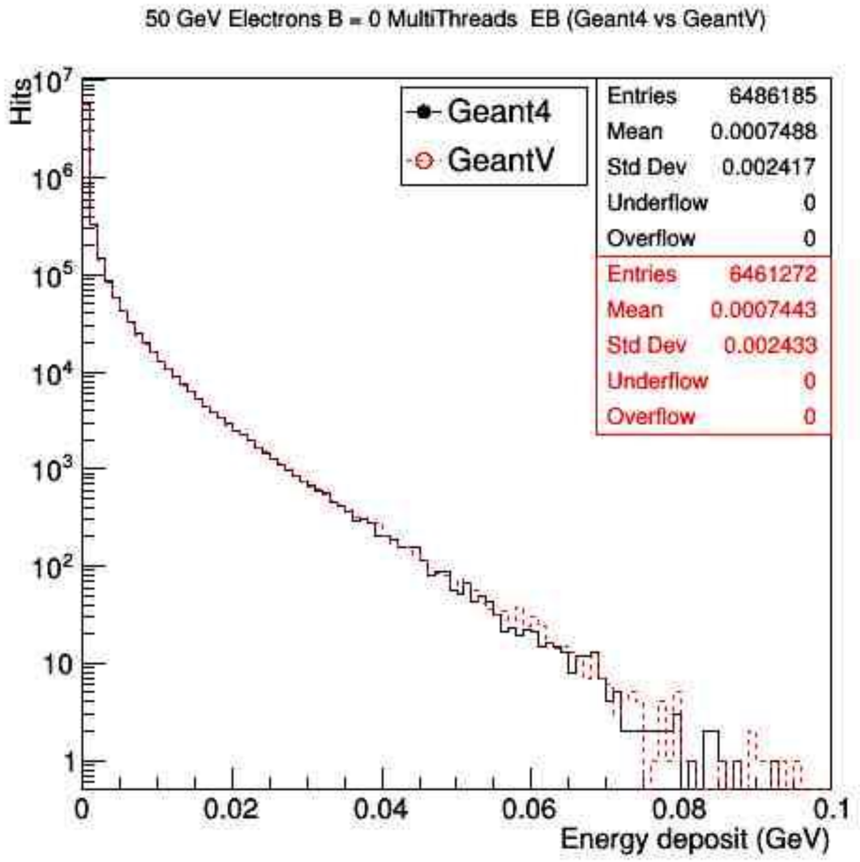


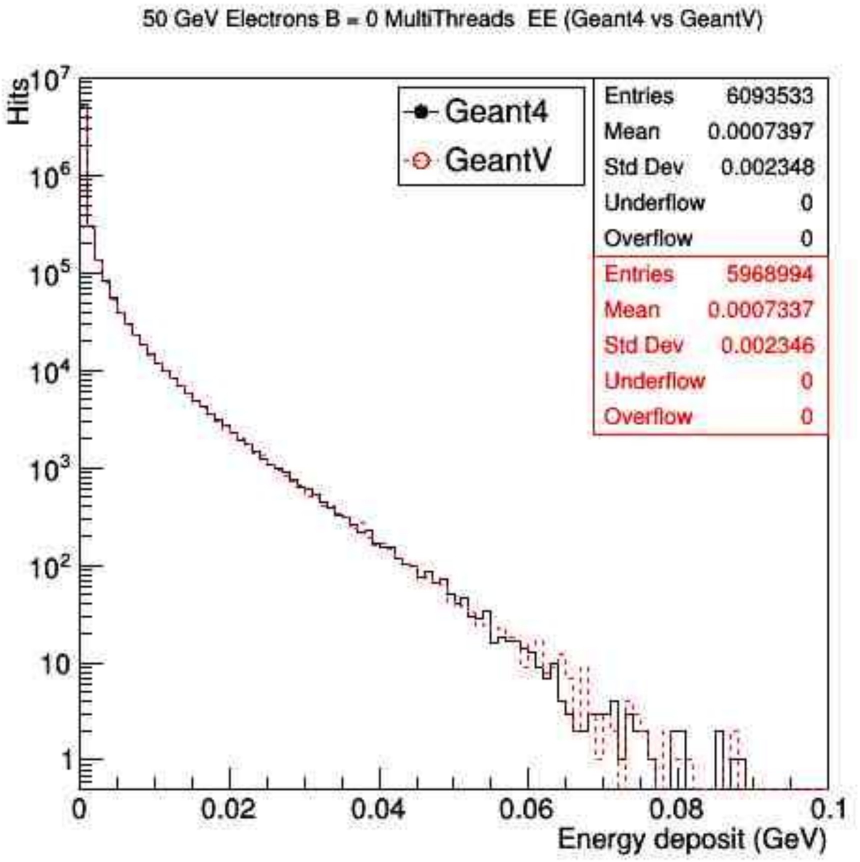
50 GeV Electrons



- Number of hits is the same for all 3 energies. The differences are at the level of 27.7/6.7/1.3% for 2, 10 and 50 GeV
- The means differ by 0.5/1.6/1.7% at the three energies

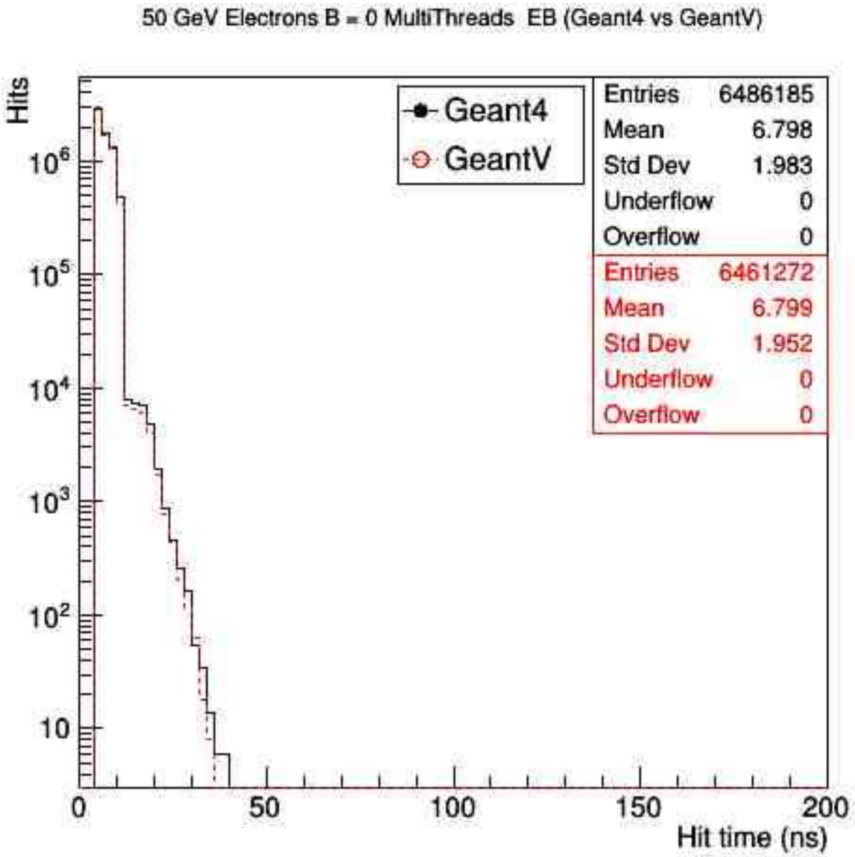
4. Energy Deposit with B = 0, MT

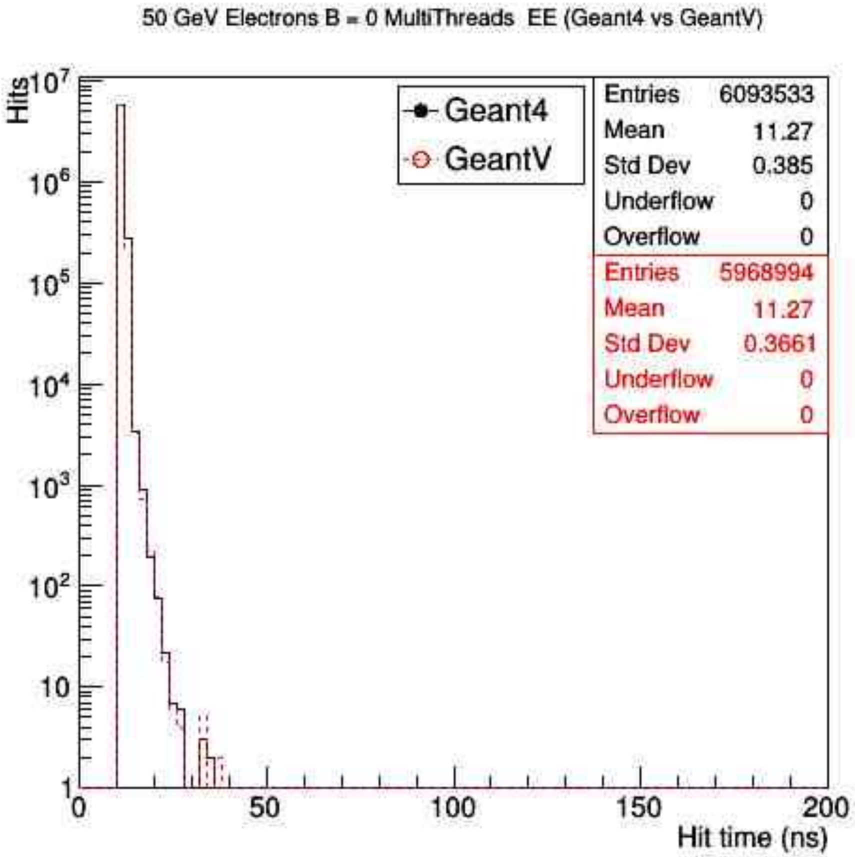




- Events are generated with 50 GeV electrons having random direction within a limited range of η and φ
- The agreement is pretty good in the B=0 option for both # of hits as well as in the shape of the distributions for EB and EE

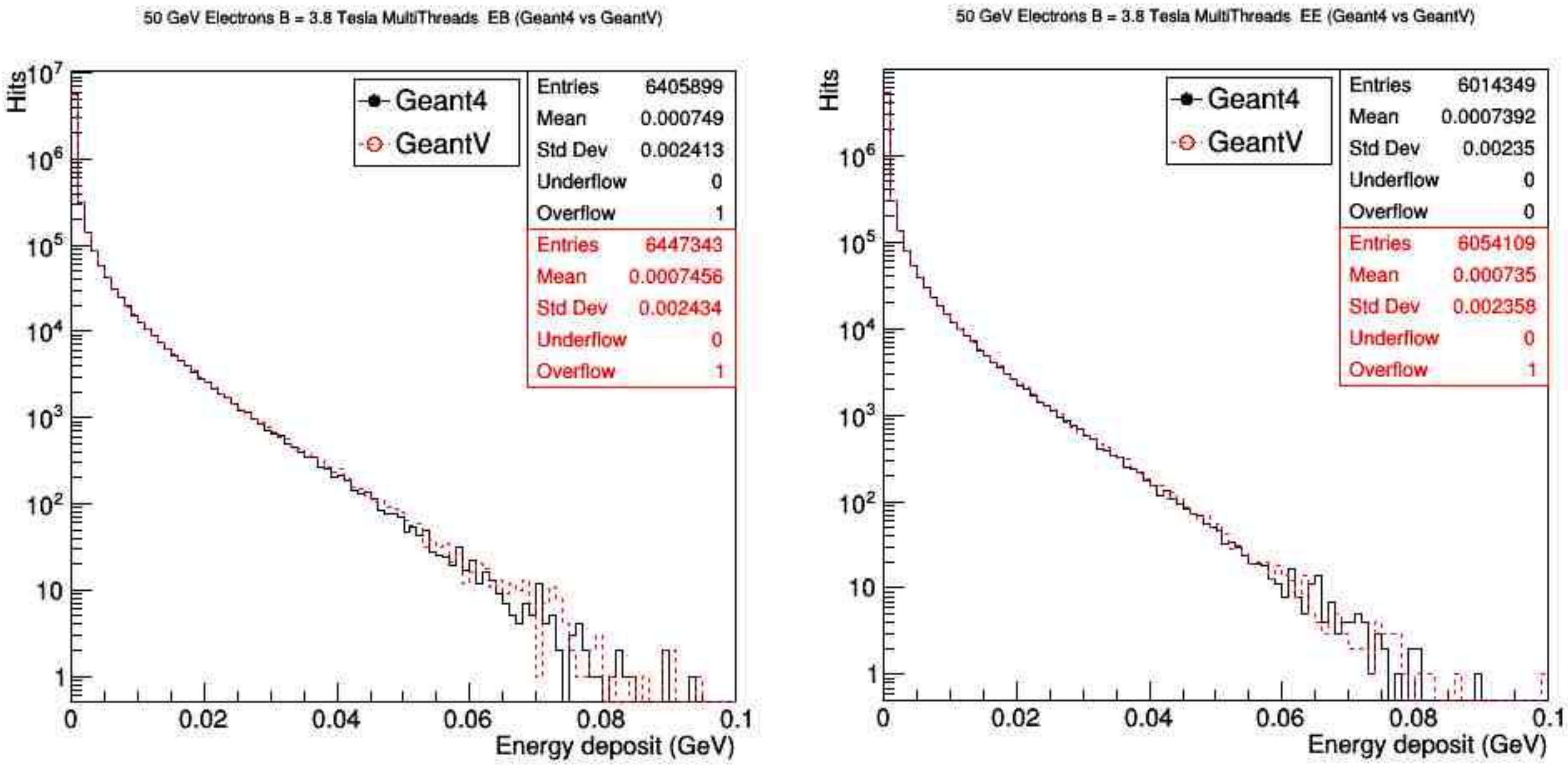
4. Hit Times with B = 0, MT





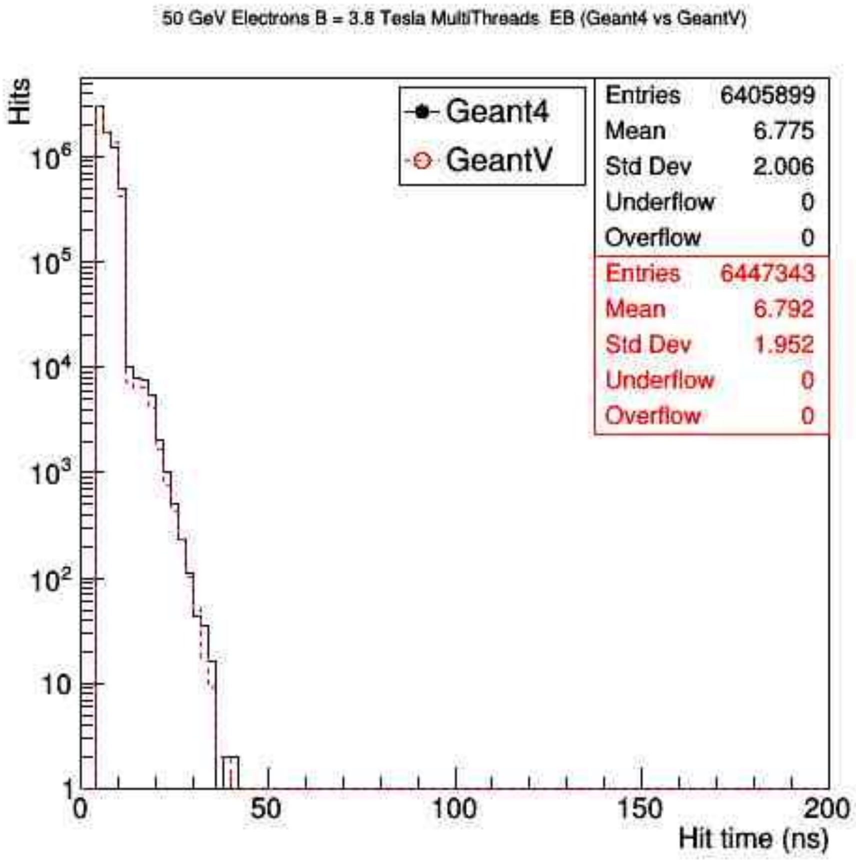
- Hit time distributions are also in good agreement for the B=0 option in EB as well as in EE

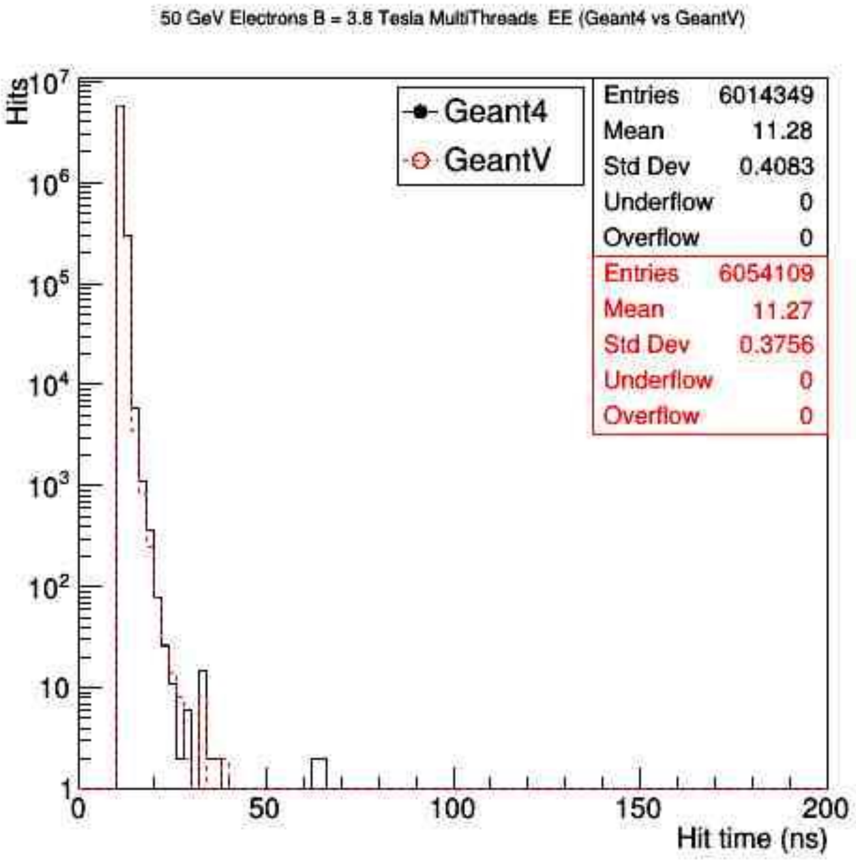
5. Energy Deposit with B = 3.8, MT



- Same events (50 GeV electrons, random direction within a limited range of η and φ) are simulated in a uniform B-field option of 3.8 Tesla
- The agreement is still good for both # of hits as well as in the shape of the distributions for EB and EE

5. Hit Times with B = 3.8, MT





- Hit time distributions are also in reasonable agreement for the B = 3.8 Tesla option in EB as well as in EE

CMS Simulation Optimizations

	Relative CPU usage	
Configuration	**MinBias**	**ttbar**
No optimizations	1.00	1.00
Static library	0.95	0.93
Production cuts	0.93	0.97
Tracking cut	0.69	0.88
Time cut	0.95	0.97
Shower library	0.60	0.74
Russian roulette	0.75	0.71
FTFP_BERT_EMM	0.87	0.83
VecGeom (scalar)	0.87	0.93
Mag. field step,track	0.92	0.90
All optimizations	0.16	0.24

- HF shower library, Russian Roulette have largest impacts
- VecGeom, mag. field improvements entered production in past ~year
  - Enabled by validating and using latest Geant4 versions
- Cumulative effects: overall, simulation is **6.2×** (**4.1×**) faster for **MinBias** (**ttbar**) vs. default Geant4 settings

➢ CMS full simulation is at least 8× faster than ATLAS