GeantV alpha-release

ANDREI GHEATA FOR THE GEANTV PROJECT

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GeantV project motivation and goals

More than 50% of WLCG power used for simulations

- The need for simulated samples will increase with luminosity

Faster full simulation & more fast simulation

- Fast simulation can help a lot up to a given point
- Full simulation still indispensable in many cases
  - Detector development and studies, simulation of the “signal” particle transport, tuning fast simulation parameters, …

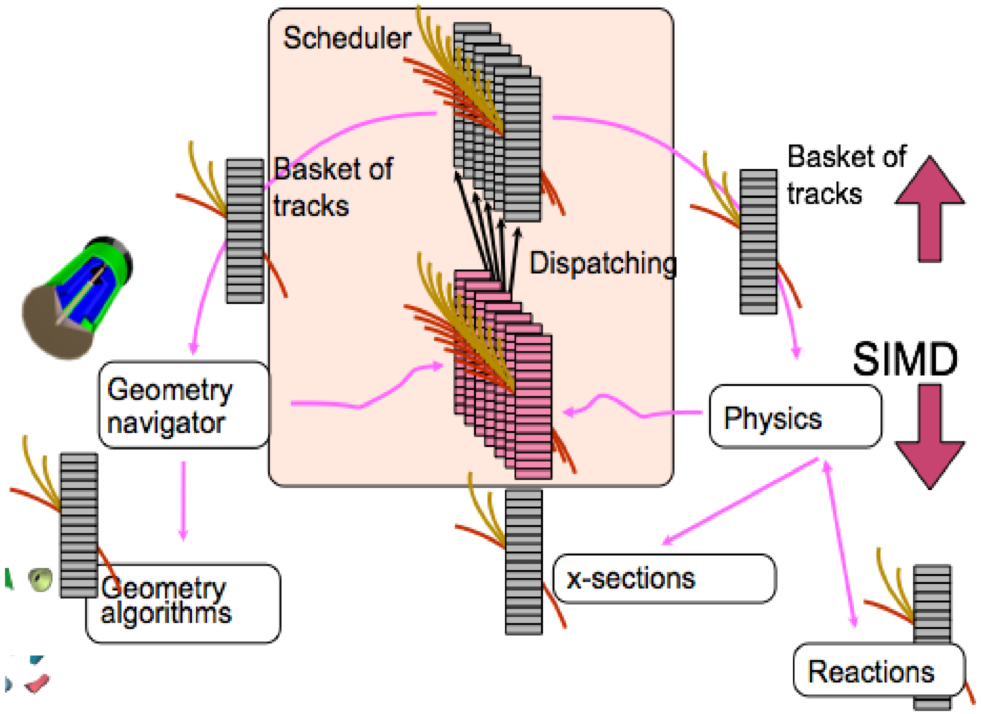
GeantV: evolve towards a faster toolkit using more efficiently CPU resources

- SIMD and NUMA topology aware, more cache friendly
- Integrate fast simulation with full simulation

Community review in fall 2016

- Deliver early a product for the community to test/adopt

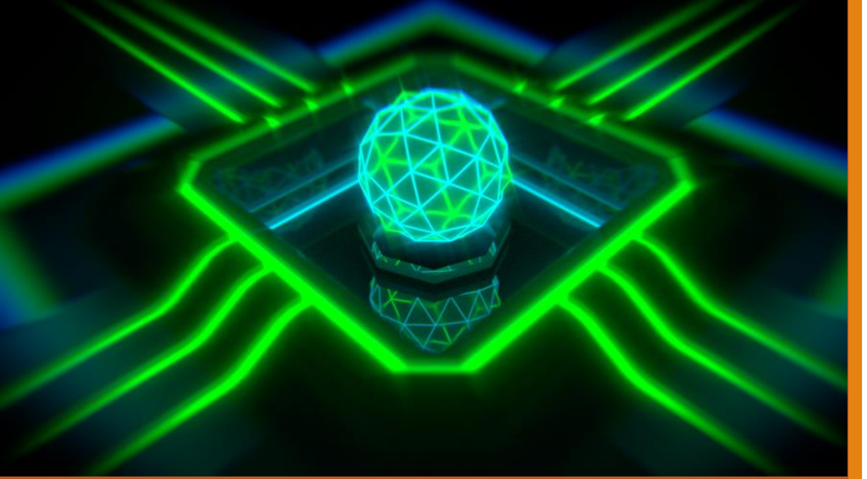
Aim for a 3x-5x faster code



Features in GeantV releases

RELEASE	CORE	USER INTRFACES	GEOMETRY	PROPAGATOR	EM PHYSICS	HADRONIC PHYSICS	FAST SIMULATION	OTHER
alpha (2017) stable interfaces allowing experiments to create own examples	v3, vectors (all) NUMA, TBB	functional	vectorized, most solids	RK vectorized	shower (e^+, e^-, γ), most processes, scalar/validated	elastic scattering validated, scalar	Simulation stage hooked in core v3	examples, demonstrators vs. Geant4
beta (2018) most of GeantV features/optimisa tions. Allowing to actually integrate experimental simulations with GeantV as toolkit	vectors (all) NUMA, TBB HPC, device[1]	finalized	vectorized, full set, fully validated	RK vectorized	shower (e^+, e^-, γ), all processes, most vectorized[2]	elastic scattering, vectorized[2] Bertini, QGS[3]	Inference from ML-based module	Reproducibility, error handling at event/track level, integration with exp. frameworks

[1] non-standard processor & GPU
[2] full assessment of vectorization potential not available for all models
[3] partial implementation

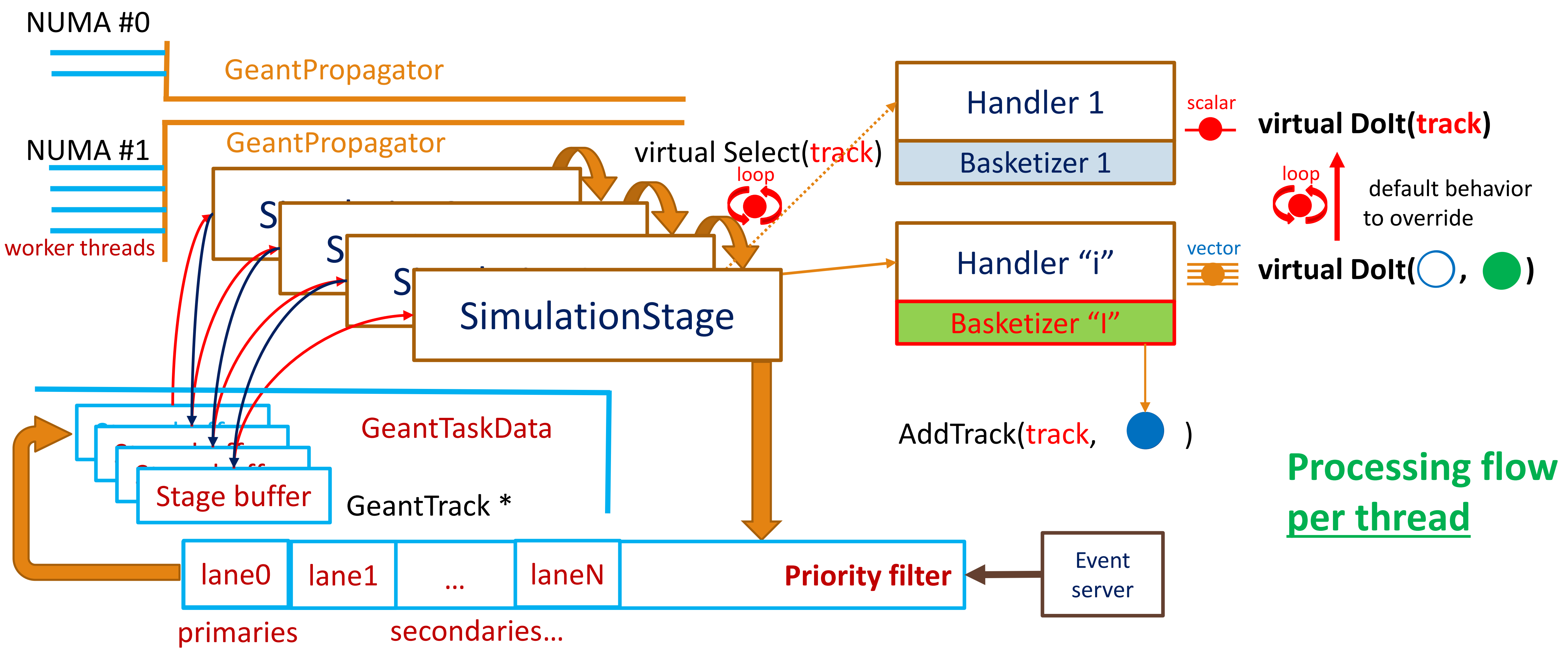


Scheduler

Orchestrating the particle flow, parallelism, topology awareness

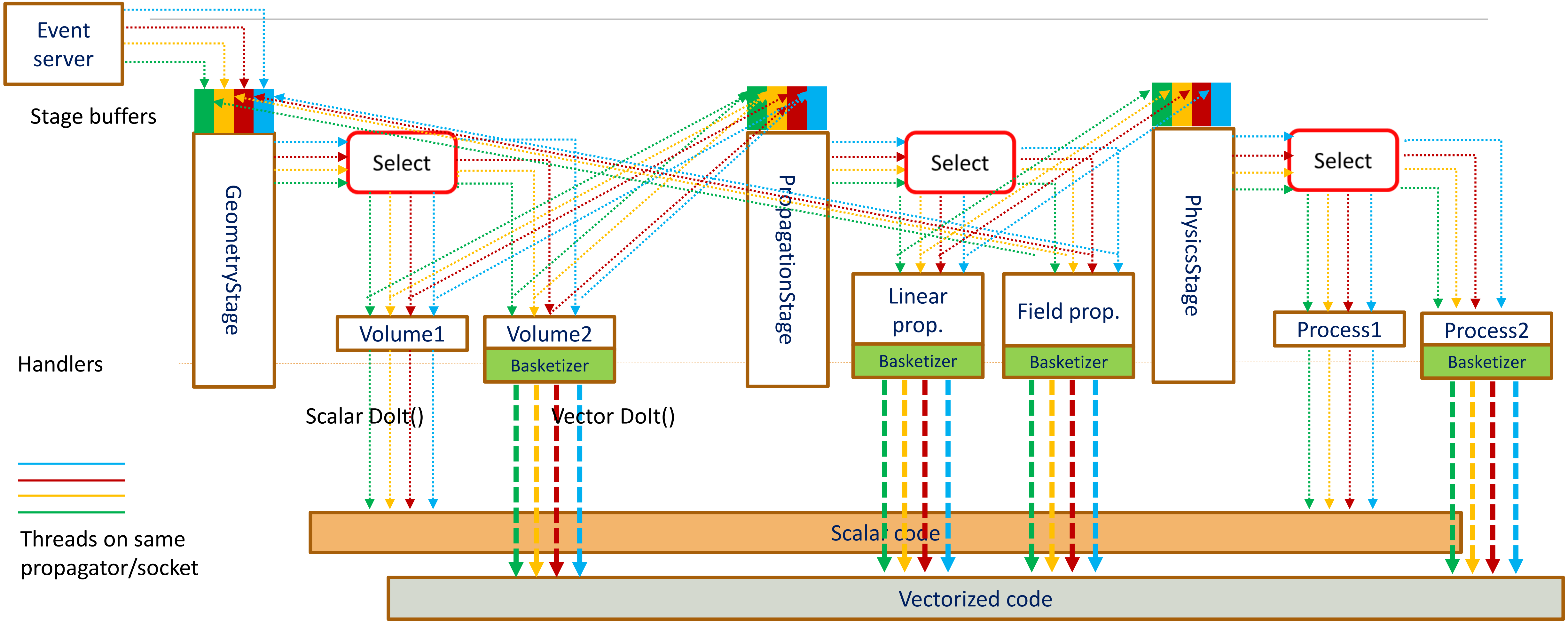
Gradually upgraded all along the R&D phase, the final version delivered in the alpha release

GeantV version 3: A generic vector flow approach

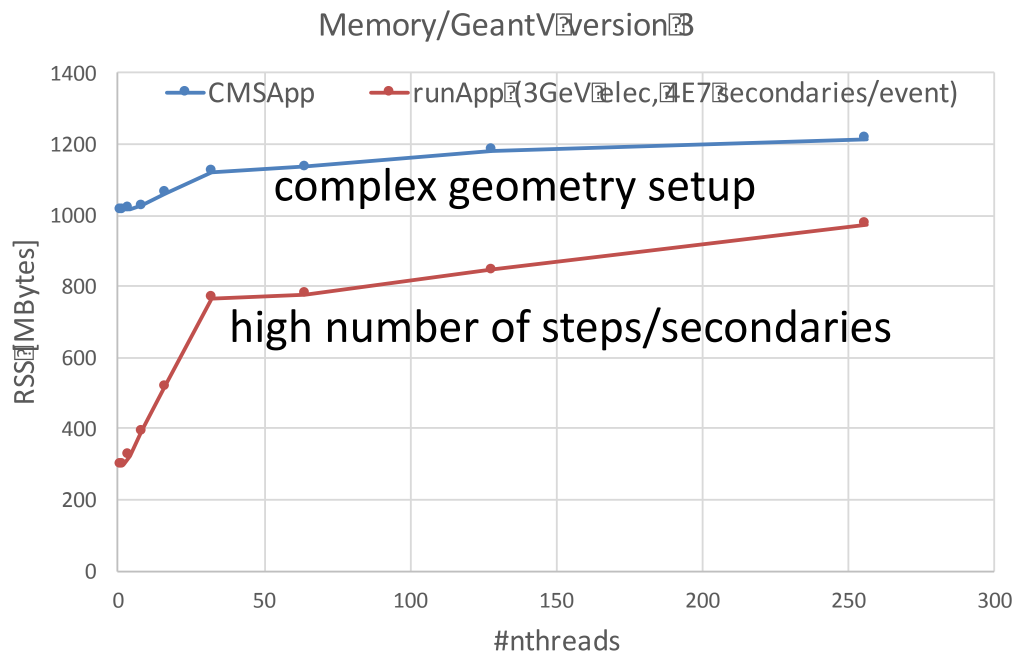


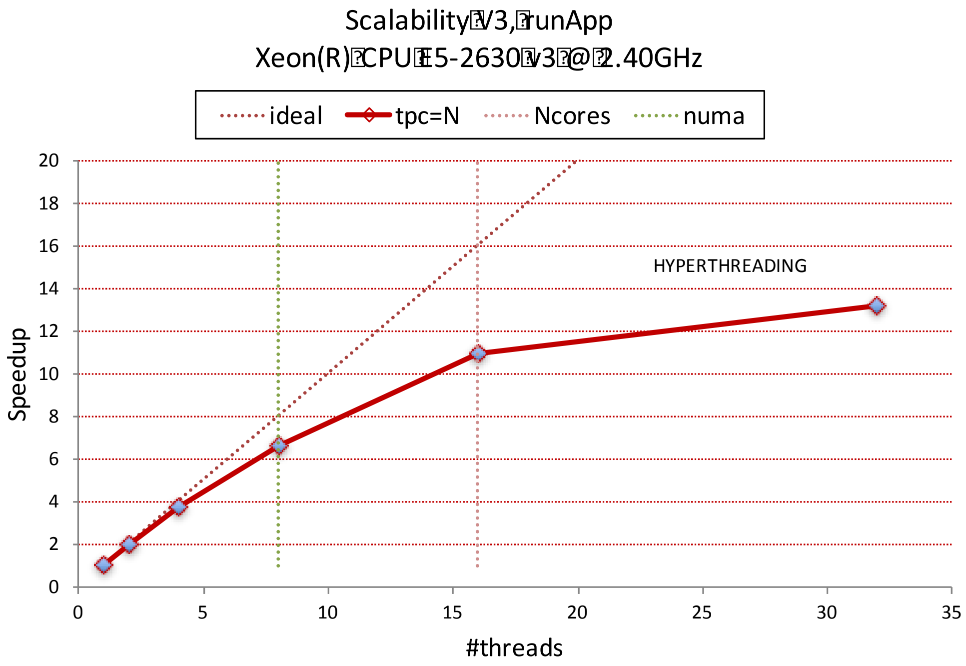
Processing flow per thread

Scalar and vector processing combined



Memory control & scalability





Stack-like control using a special filter inserted in the stepping loop preventing bulking the memory

- Higher generation secondaries flushed with priority

No difference in profile for N/2N threads

- Memory operations are high in the profile, expected to improve when having more (vector) work on physics side

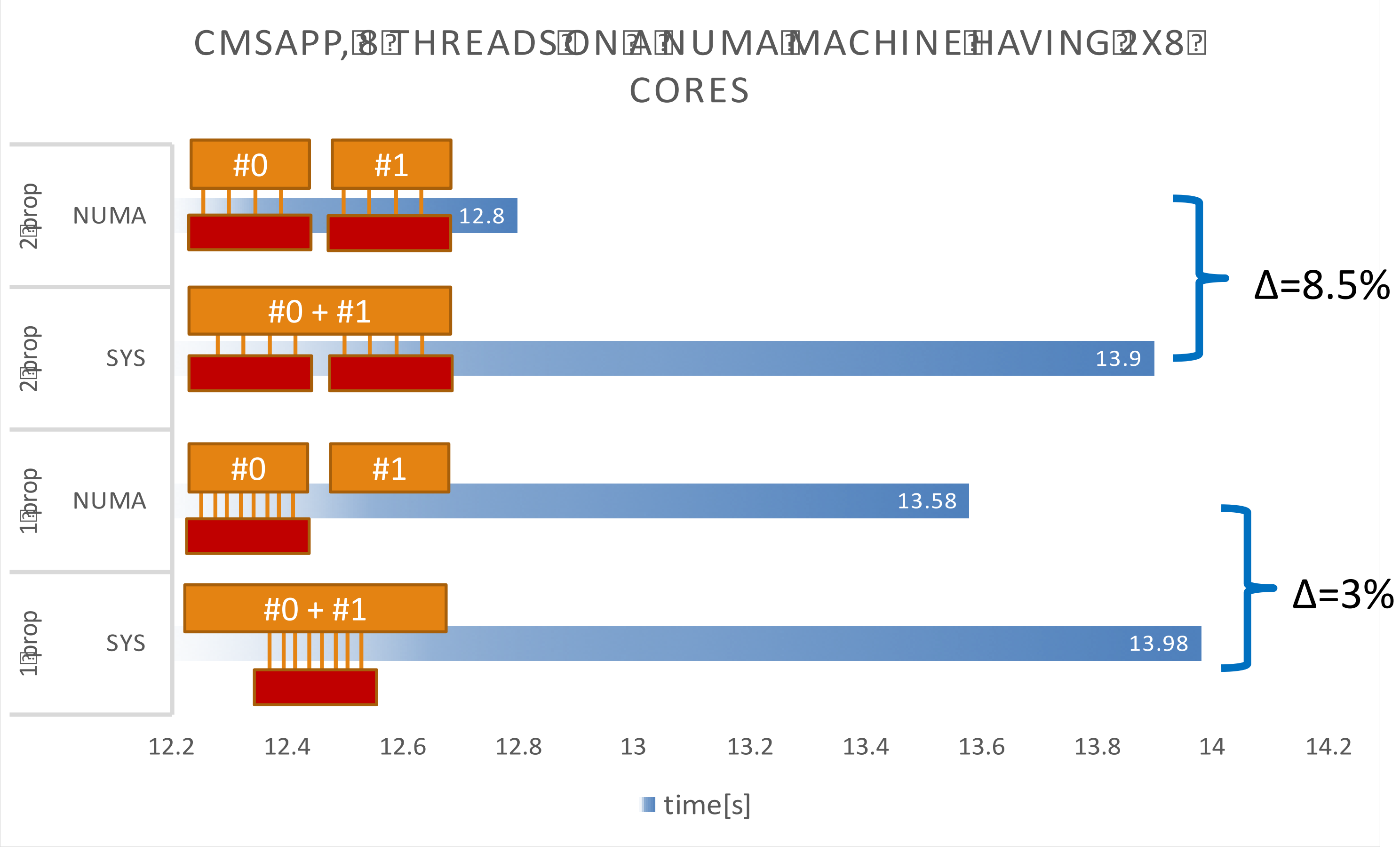
NUMA awareness versus OS policy

NUMA mode

- Topology detection using *hwloc*
- A propagator will use threads bound to the same NUMA node
- One or more propagators per NUMA node

Allocation policy

- Threads – compact binding
- Propagators – scattered binding
- Memory – track blocks and buffers pinned to NUMA nodes



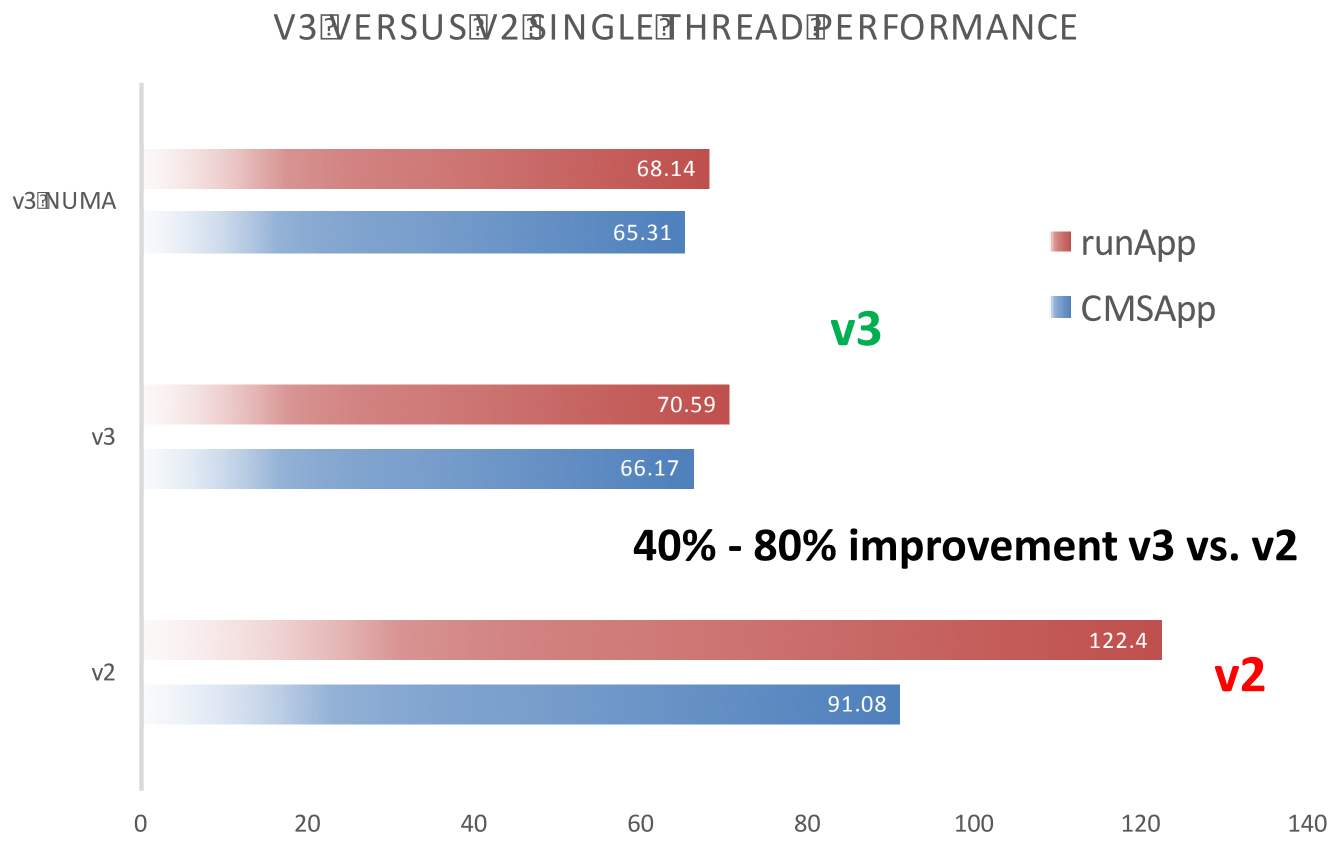
Overall single thread improvement

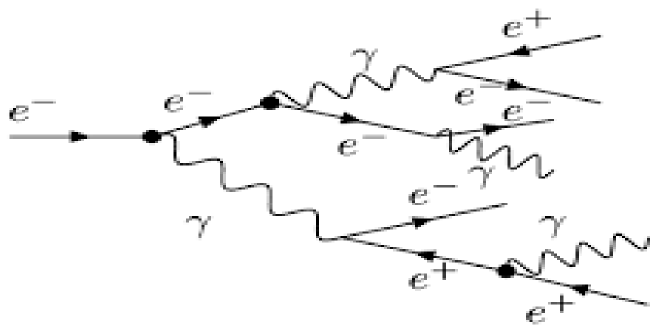
Comparing new and old version of GeantV with same benchmarks

- Vector interface with geometry not activated

Assessment/projections of speed performance compared to Geant4 will be done for a set of benchmarks in the alpha release

- Different geometry complexity and physics settings, magnetic field on/off, vectorization on/off





EM physics

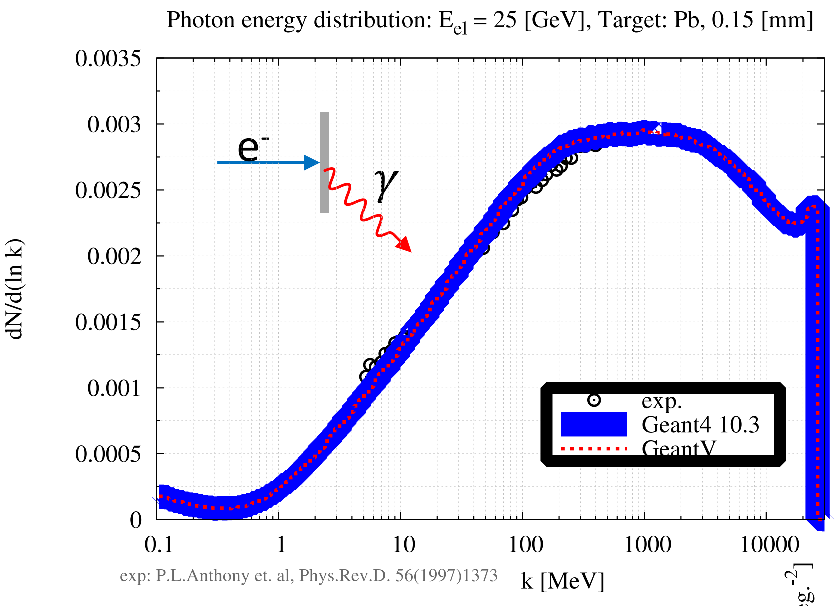
Deliver full EM shower, initially in scalar mode in the alpha

GeantV EM physics status

* under development

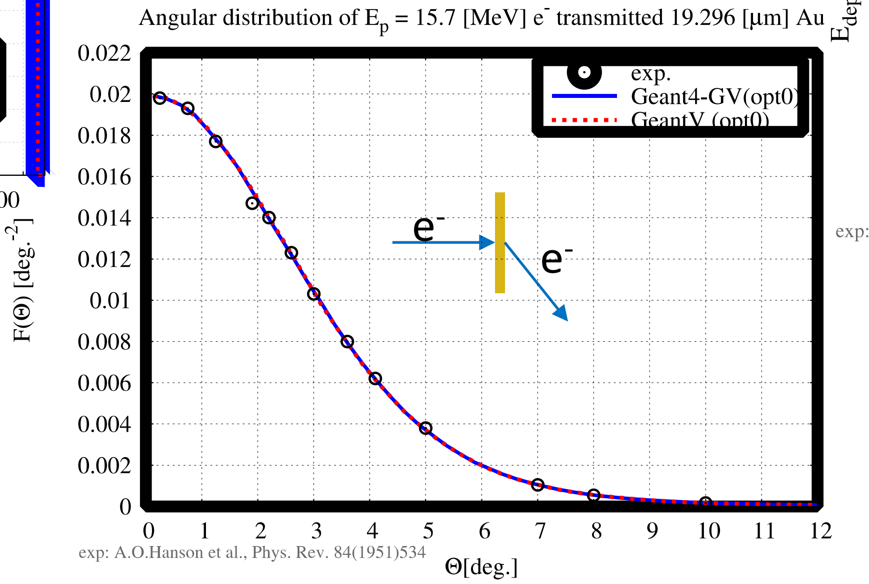
particle	processes	models(s)	
		GeantV	Geant4
e^-	ionisation	Møller[100eV-100TeV]	Møller[100eV-100TeV]
	bremsstrahlung	Seltzer-Berger [1keV-1GeV]	Seltzer-Berger [1keV-1GeV]
		Tsai (Bethe-Heitler) w. LPM. [1GeV-100TeV]	Tsai (Bethe-Heitler) w. LPM. [1GeV-100TeV]
	Coulomb sc.	GS MSC model [100eV-100TeV]	GS 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]	GS MSC model [100eV-100TeV]
			Mixed model [100MeV-100TeV]
	annihilation	-	Heitler (2γ) [0-100TeV]
γ	photoelectric	new Livermore (*)	SANDIA par. [100eV-100TeV] + deEx.
	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

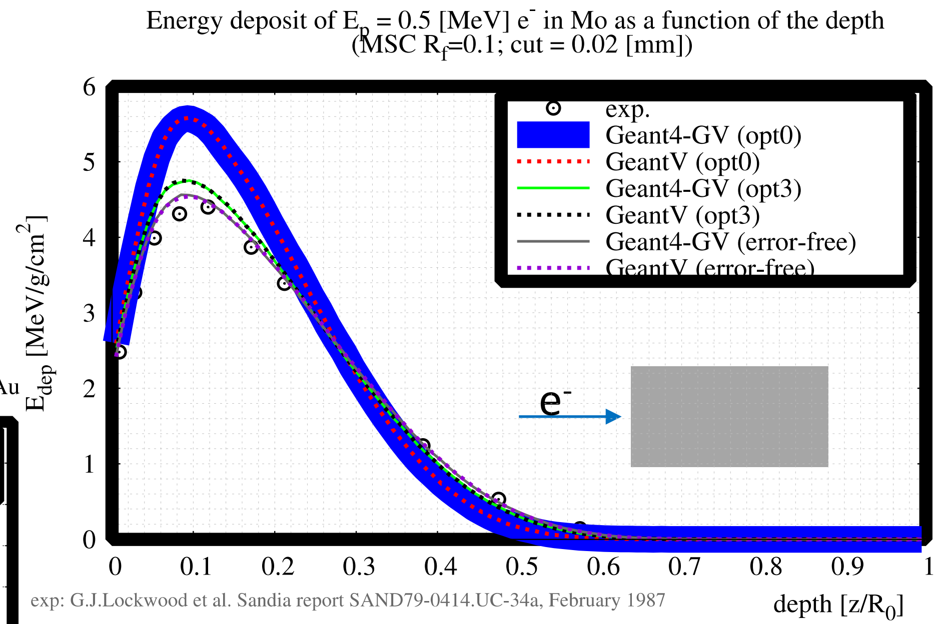
EM Physics validation



Thin layer, bremsstrahlung test

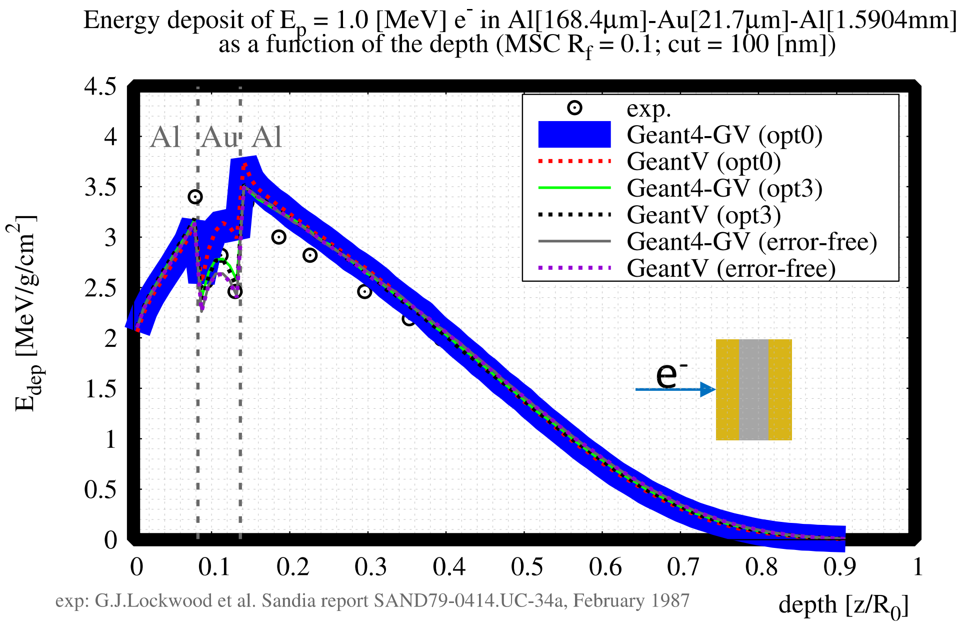
Thin layer, MSC test





Semi-infinite block, MSC test

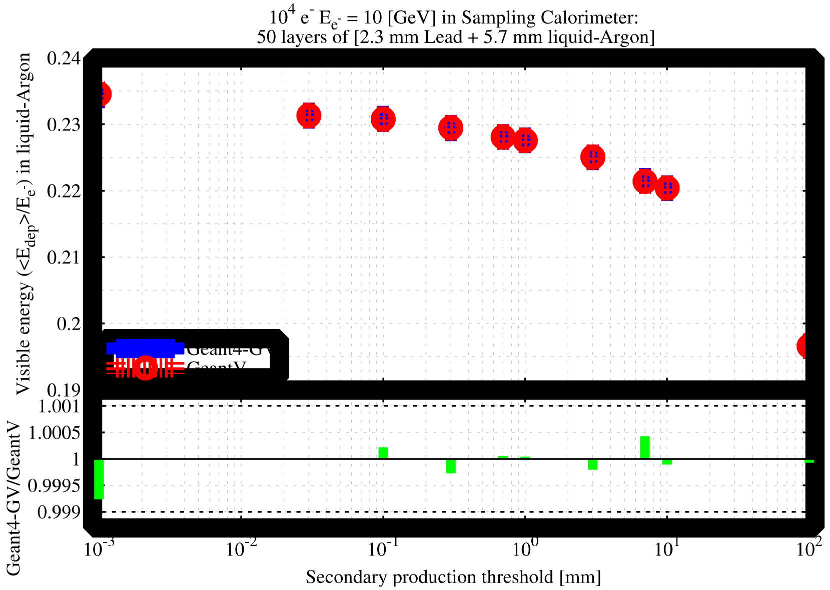
EM Physics validation



Multi-layered target

10^5 1 [GeV] e- in ATLAS bar. simpl. cal. : 50 layers of [2.3 mm Pb + 5.7 mm lAr]; p.cut = 0.7 [mm]

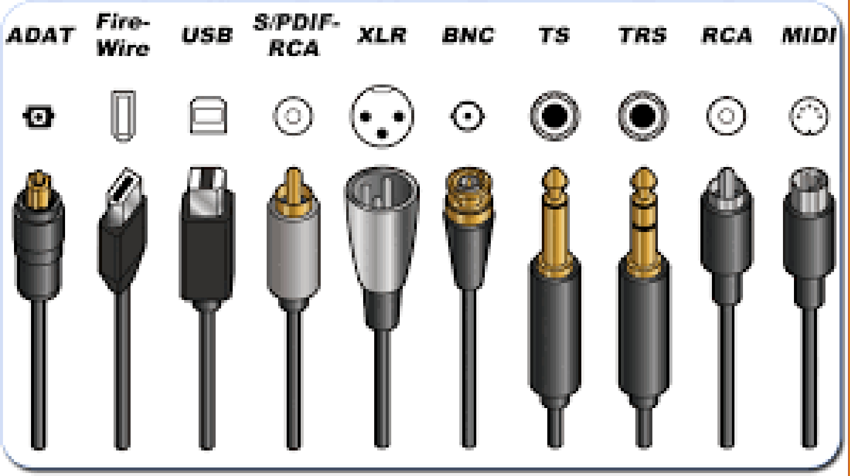
	e^-/e^+: ionisation, bremsstrahlung, msc; γ: Compton, conversion							
	GeantV				Geant4			
material	E_d[GeV]	rms [MeV]	tr.l. [m]	rms [cm]	E_d[GeV]	rms [MeV]	tr.l. [m]	rms [cm]
Pb	0.69450	15.198	51.015	1.189	0.69448	15.234	51.016	1.192
lAr	0.22792	14.675	106.11	7.592	0.22796	14.656	106.13	7.582



Mean number of :

gamma	405.87	406.15
electron	9411.49	9419.44
positron	53.77	53.71
charged steps	11470	11476
neutral steps	49177	49222

ATLAS simplified sampling calorimeter



User Interfaces

Complete set of interfaces and a set of examples demonstrating their usage in the alpha

User interfaces – impact on user framework

Similarities with Geant4:

- User detector construction, generator
- Scoring interfaces

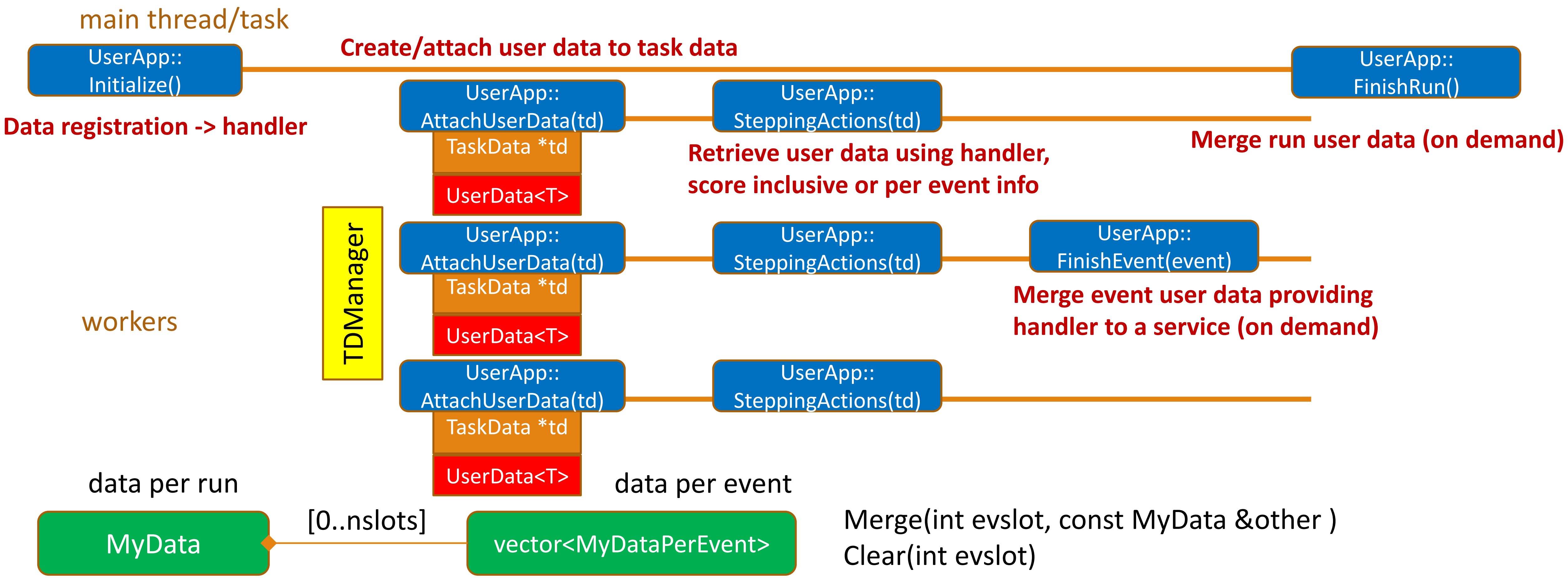
New features:

- Concurrent scoring, limited number of events in flight
- Multi-particle interfaces, tracks from multiple events mixed
- Data structures per thread and per event + merging

GeantV support:

- Examples demonstrating efficient data access patterns
- On-demand merging service
- Hit factory & concurrent I/O
- Task-based parallelism support and example of external event loop - ongoing

Example: concurrent scoring (transient)



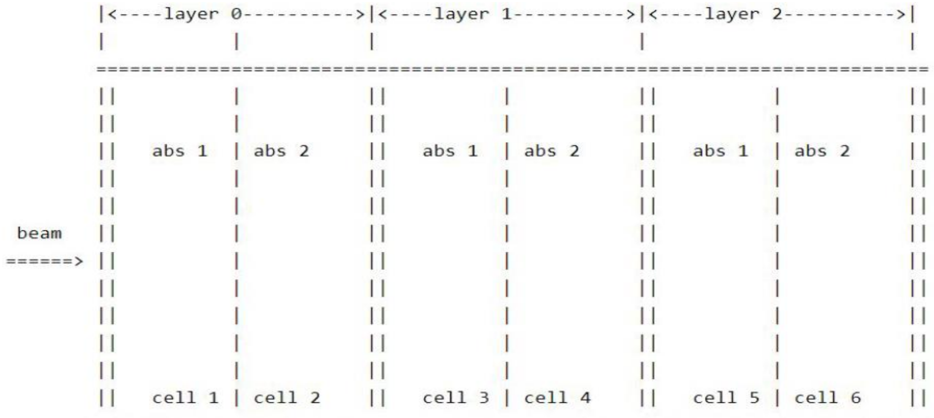
User application: examples

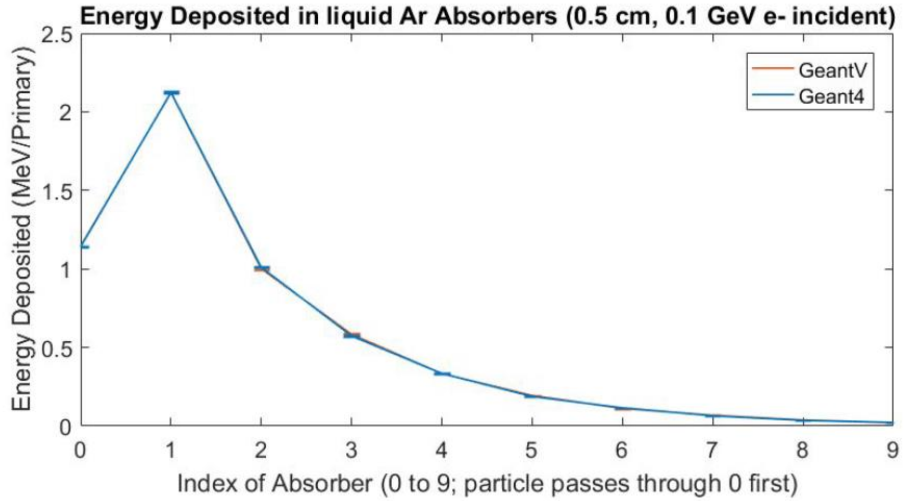
Fully configurable GeantV example applications

- Including configurable user defined detector construction, geometry, physics list with custom physics process, primary generator
- Showing how to do scoring
- Geant4 equivalent also demonstrated and compared

Current examples

- Simple calorimeter
- More examples being prepared





R&D

Several ongoing sub-projects, preparing new features for the beta and beyond

ML prototype for fastsim in the alpha

S. Vallecorsa
16:45 Track 1 today

Fast simulation "hooks" à la G4 designed according to v3 flow

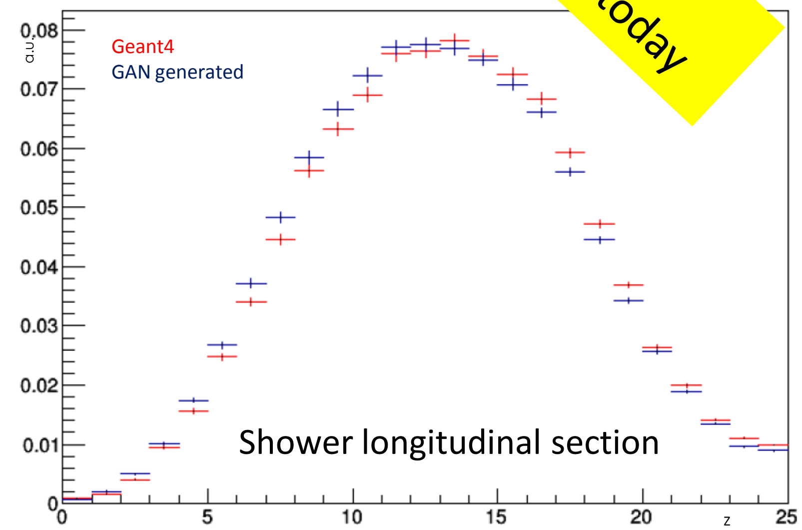
- First implementation of the user interfaces

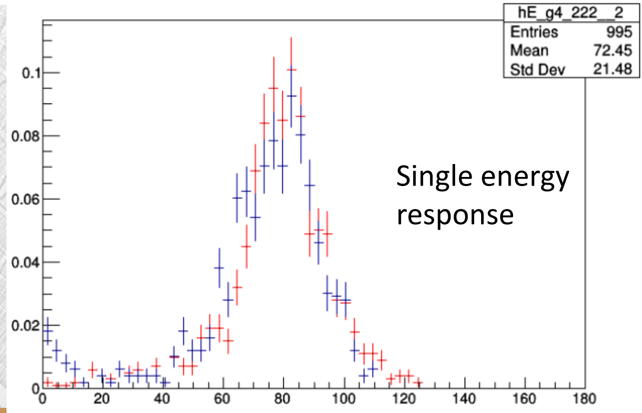
First ML prototype for simulation of high granularity calorimeters

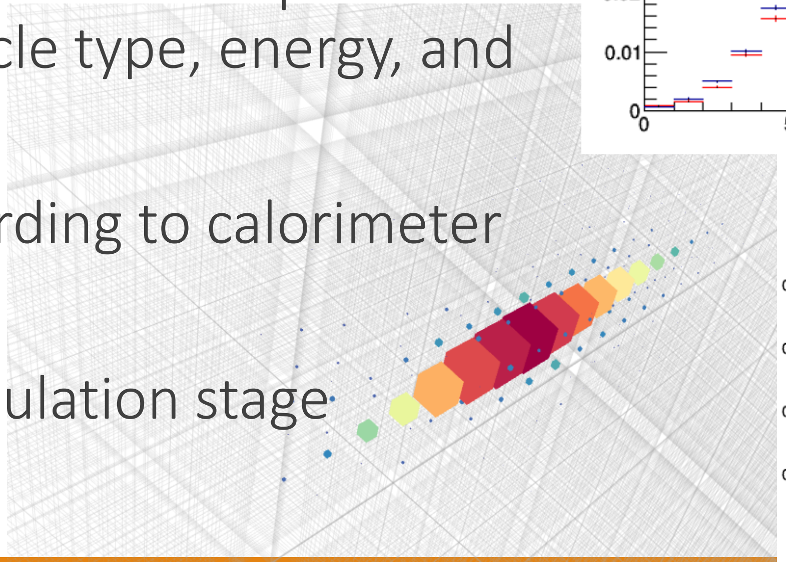
Complete GAN based model for the simulation of particle showers in calorimeter (including particle type, energy, and trajectory)

First algorithm meta-optimization according to calorimeter geometry

Integration of the inference step as simulation stage

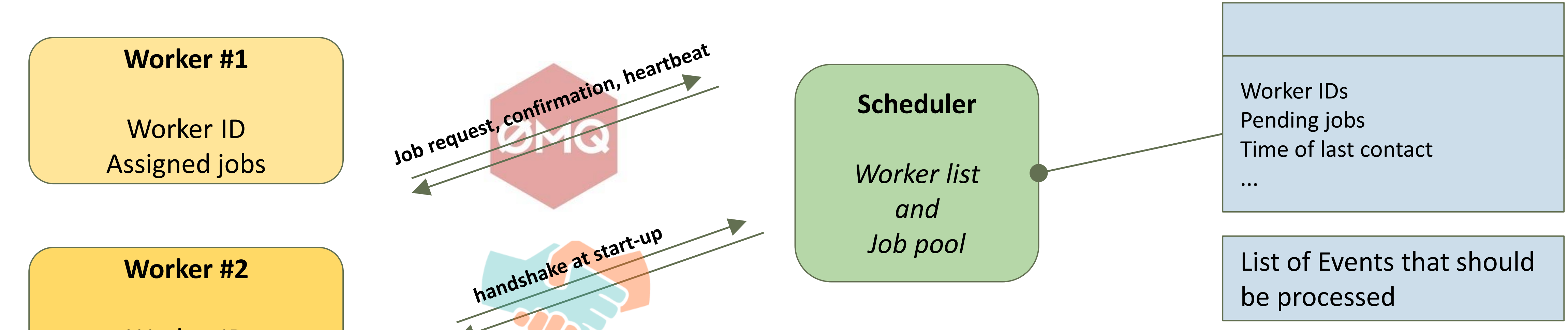


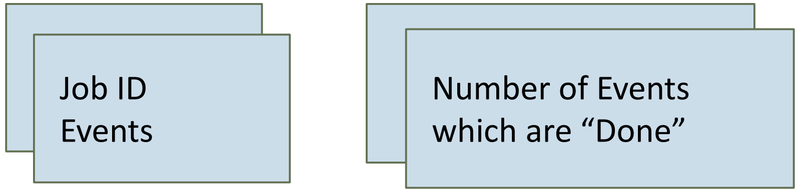




100 GeV electrons

GeantV HPC mode



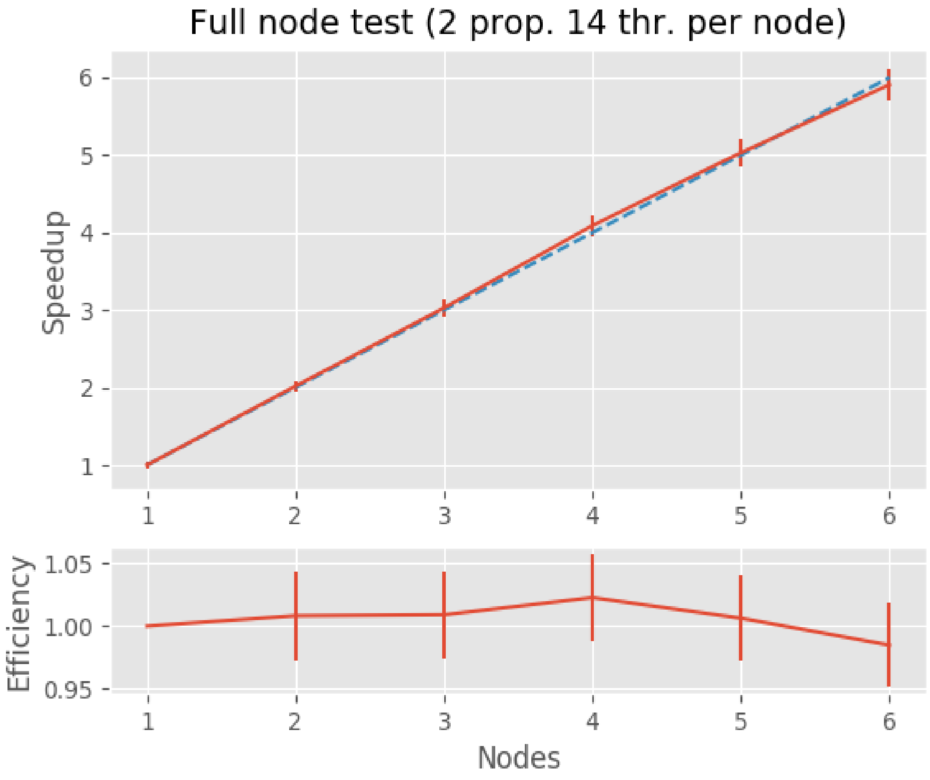


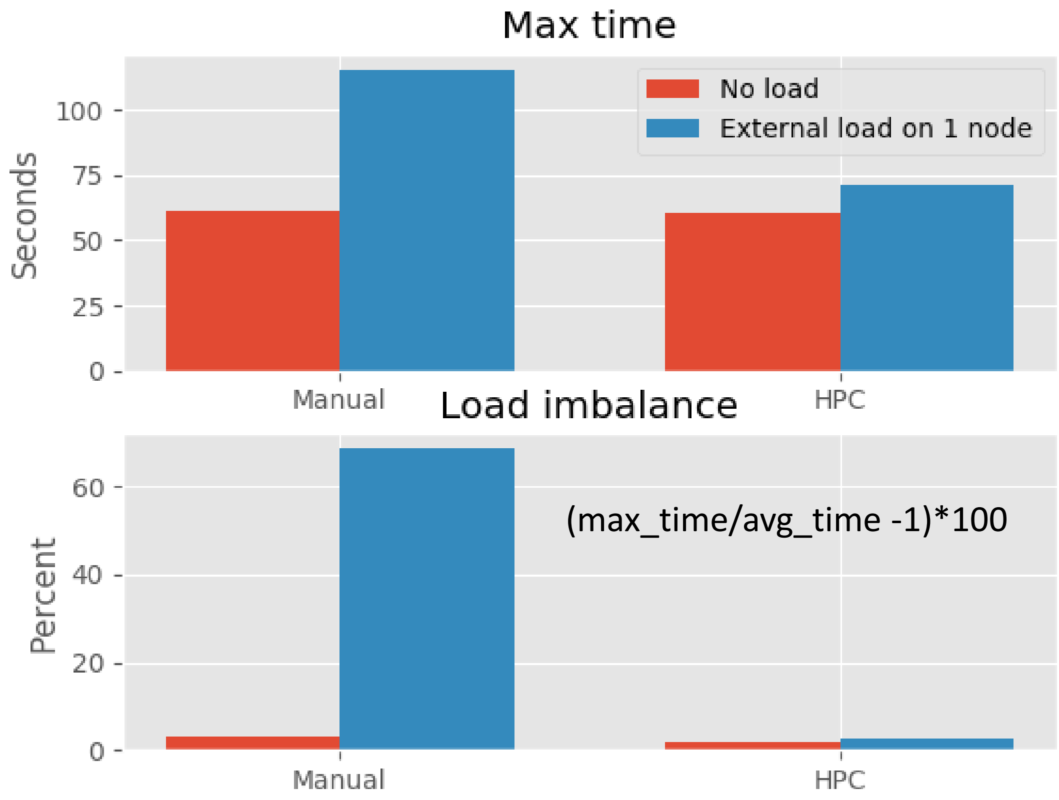
Applicable to other CPU-bound applications than GeantV

***Going beyond data parallelism*:**

- Scheduling the work from the application
- Optimizing work per machine using topology discovery;
- Handle un-even load, policies for work (re)distribution
- Resilience to hanging/dead workers

GeantV HPC mode: preliminary results





Outlook

GeantV developments on a tight schedule towards the end-of-year release

- Program of work became much more focused on releases
- Most components almost ready (core, EM physics, interfaces & examples), others still under development (field propagation, hadronic physics, more complex examples with new EM physics, complete flow including GPU)

The alpha release will feature mainly shower EM physics

- Delivering part of the design performance (vectorized geometry but scalar physics)
- Interfaces mature enough to make the product usable by experiments for testing
- Many more features and design performance expected in the beta version

Important R&D still ongoing

- Event loop steered by user application + CMSSW demonstrator
- Generic fast simulation approach + integration as simulation stage
- GeantV optimization for HPC

Thank you !