FEDERICO CARMINATI

JAN 25, 2016

SIMULATION POW 2016

DISCLAIMER

- Items are NOT in order of priority
- People are NOT in order of importance
- People mentioned on the same task may NOT contribute to it at the same level
- I focused on the SFT work, FNAL contribution is not properly described

THE SIMULATION TEAM 2016

- Ananya🌷, J.Apostolakis, M.Bandieramonte, G.Cosmo, G.Folger, M.Gheata✨, A.Gheata(intel), I.Goulas, F.Hariri, D.Konstantinov⚽, H.Kumawat🎄, V.Ivantchenko, T.Nikitina, M.Novak, W.Pokorski, A.Ribon, R.Seghal🎄, O.Shadura, S.Vallecorsa(intel), S.Wenzel✨)
- People who left😢: A.Arora🌷, A.Bhattacharyya🎄, Y.Zhang
- People leaving😢: Ananya🌷 (Mar 16), R.Seghal🎄 (Sep 16), S.Wenzel✨(Mar 16)
- People arrived😊: Ananya🌷, A.Arora, D.Konstantinov, M.Bandieramonte, M.Gheata✨, R.Seghal🎄, Y.Zhang, S.Vallecorsa(intel)
- People arriving😊: H.Fariri (Fellow, Mar 16), H.Kumawat🎄(Mar 16)

✨AIDA 😊 🎄BARC 😊 🌷IIT Mumbai 😊 ⚽Genser 😊

ACHIEVEMENTS 2015

GEANT4 HADRONIC PHYSICS

- Refactoring of hadronic XS code for better maintainability (W.Pokorski)
  - Code & doc review, migration to Glauber-Gribov model reproducing k asymmetry observed by LHCb
- Further upgrade of de-excitation module: physics, CPU, memory (V.Ivantchenko)
  - Release of new model of nuclear gamma de-excitation based on the same database as radioactive decay
- Overhaul of the QGSM model (A.Ribon with V.Uzhinskii)
  - Improvements to the string model (FTF & QGS) codes

GEANT4 ELECTROMAGNETIC PHYSICS

- Web-based tools to handle EM testing suite (A.Bagulya, V.Ivantchenko)
  - Web interface to the data in afs (revival & update of an old code)
- Maintenance of EM package focused on LHC (V.Ivantchenko)
  - Completed EM migration to MT (including PAI)
  - Simpler steering of EM parameters
- Kawrakow-Bielajew Goudsmit-Saunderson & PENELOPE multiple scattering models (M.Novak, V.Ivantchenko)
  - Improved and extended models for single and multiple scattering
  - Goudsmit-Sanderson for e-/e+ MS, theory based & better accuracy and speed

GEANT4 GEOMETRY

- Review and improvement of safety calculation in MT (J.Apostolakis)
  - Postponed to 2016
- Issues from ALICE geometry, ATLAS & g-2 transport (J.Apostolakis)
  - Ffixed it (the effort needed is the reason for the postponements!!)
- Multi solid-type parameterisations in MT (J.Apostolakis, G.Cosmo)
  - Enabled multi-threading for any kind of volume parameterisations and divisions
- Improved verbosity in Navigation (to aid in debugging) (J.Apostolakis, G.Cosmo)
  - Done
- Parallel Navigation - performance / robustness (J.Apostolakis)
  - Postponed 2016
- Replace Usolid shapes with VecGeom ones and test them with Geant4 (G.Cosmo, T.Nikitina, FNAL)
  - Implemented and extended new interface to VecGeom/USolids as external independent library

GEANT4 SERVICES

- Support for GDML, ROOT I/O (W.Pokorski, G.Cosmo)
  - New GDML version with extended module and schema to support (also) regions&cuts
  - Geometry persistency for Geant 10 (MT) & ROOT 6
- Release coord, building & installing, nightly & cont testing (G.Cosmo, G.Folger)
  - Rel 10.2 & monthly ref tags (afs & cvmfs, 9.6.p04, 10.0.p04, 10.1.p01, 10.1.p02)
  - Set up puppet based machines
  - Asked LHC for a “reasoned schedule” of releases – conclusion: our schedule is *perfect* 😀

GEANT4 SERVICES

- Coordination of the C++11 task-force (G.Cosmo – coord, W.Pokorski, G.Folger)
  - Defined strategy for migration to selected C++11 features & started implementation
- Migration of Geant4 web to Drupal (G.Folger)
  - Test site setup, mirroring tested… will be finished in 2016
  - G4 tagsdb migrated from Drupal to afs webserver
  - tagsdb web interface tested – expected 1Q16
- Migration to Jenkins (G.Folger, O.Shadura, P.Mendez Lorenzo)
  - Done including nightly & continuous, new platforms and support to shifters

OTHER PROJECTS

- Coordination of GENSER (W.Pokorski, D.Konstantinov)
  - Regular releases of MC generators integrated with LCG external software
- Coordination of HepMC3 development (W.Pokorski, D.Konstantinov)
  - Beta releases for experiments test
  - Improvement of ROOT I/O
- Validation DB (W.Pokorski, A.Ribon, D.Konstantinov, G.Folger)
  - Review & re-implementation of the validation DB@FERMILAB
  - Implementation of API allowing applications to directly access the DB

OTHER ACHIEVEMENTS

- Grid testing and validation (G.Cosmo, W.Pokorski, D.Kostantinov)
  - Monthly tag validation campaigns (published on web service http://g4-val.cern.ch)
- Field stepper (J.Apostolakis)
  - GSoC student development of high order Runge-Kutta (reduction of up to 20-40% in # of calls)
- Random number generator (G.Cosmo)
  - Review of existing methods and introduction of MixMax engine, interfaced to CLHEP
- Code maintenance (G.Cosmo)
  - Coordinate & contribute to cleanup of coverity defects & check for unending loops
- CMS production with Geant4 10.0p03+patches MT (V.Ivantchenko)
  - Coordinated CMS-sim releases, used to produce ~8 B G4 events@13 TeV
  - New Geant4 10.1 and 10.2 tested within CMSSW

GEANTV THE BIG PICTURE

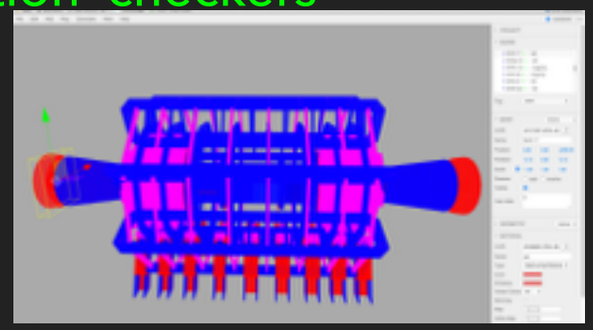
- Demonstrate substantial speedup for a LHC-size detector by 2H15 with the following features
  - Functional navigation 😀
  - Full tabulated physics 😀
  - Generator interface 😀
  - Vectorised e-gamma ☹️
  - I/O of hits, digits & kinematics 😐
  - Working on x86, Xeon Phi (acc / full port), NVIDIA (acc) 😐
  - Vectorised Multiple Scattering and Mag field transport 😐
  - Example of “fast MC” ☹️
  - Code repo, build & test environment 😀

GEANTV SCHEDULER

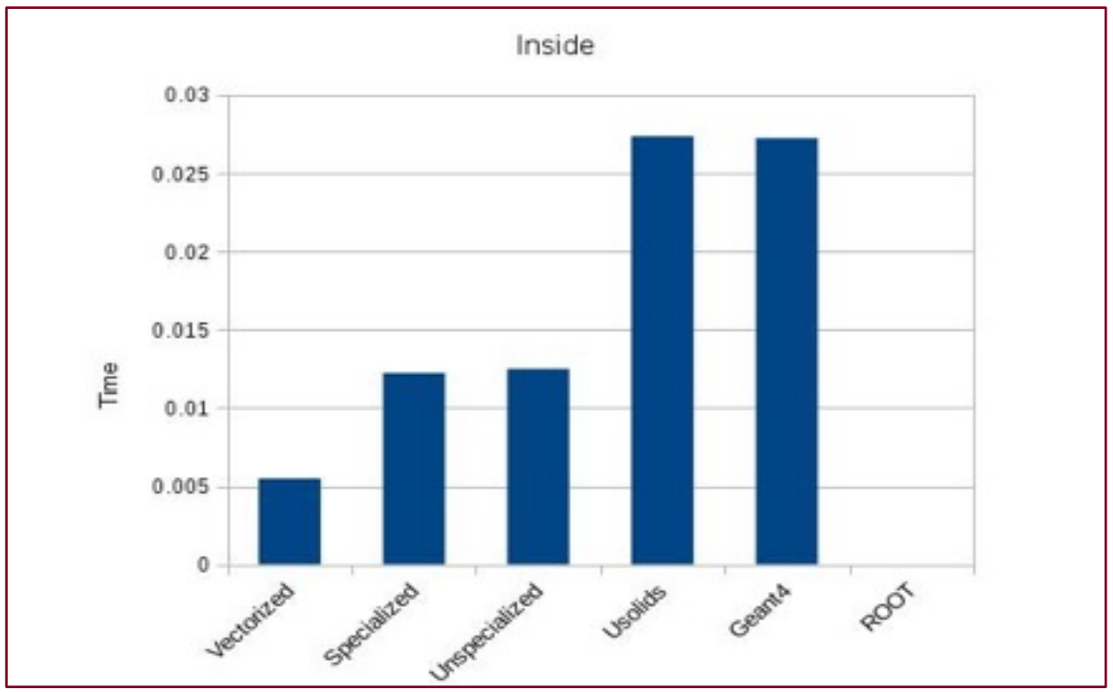
- Improve CPU/GPU synchronisation mechanism (FNAL, A.Gheata, S.Wenzel)
  - Major process in this area, tracks & geometry can be exchanged
- Redesign of concurrent basket filling, reduce contention & memory footprint (FNAL, A.Gheata)
  - Done, see next slides
- Concurrent hits and digits (A.Gheata, W.Pokorski)
  - Concurrent output “hits” with TMemoryFiles merging, good scaling with number of threads
- Kinematics format and I/O (A.Gheata, W.Pokorski)
  - Interface to generic HepMC3 event input
- Investigate data structures: SOA⇔AOSOA (FNAL, A.Gheata, S.Wenzel)
  - Done, see next slides

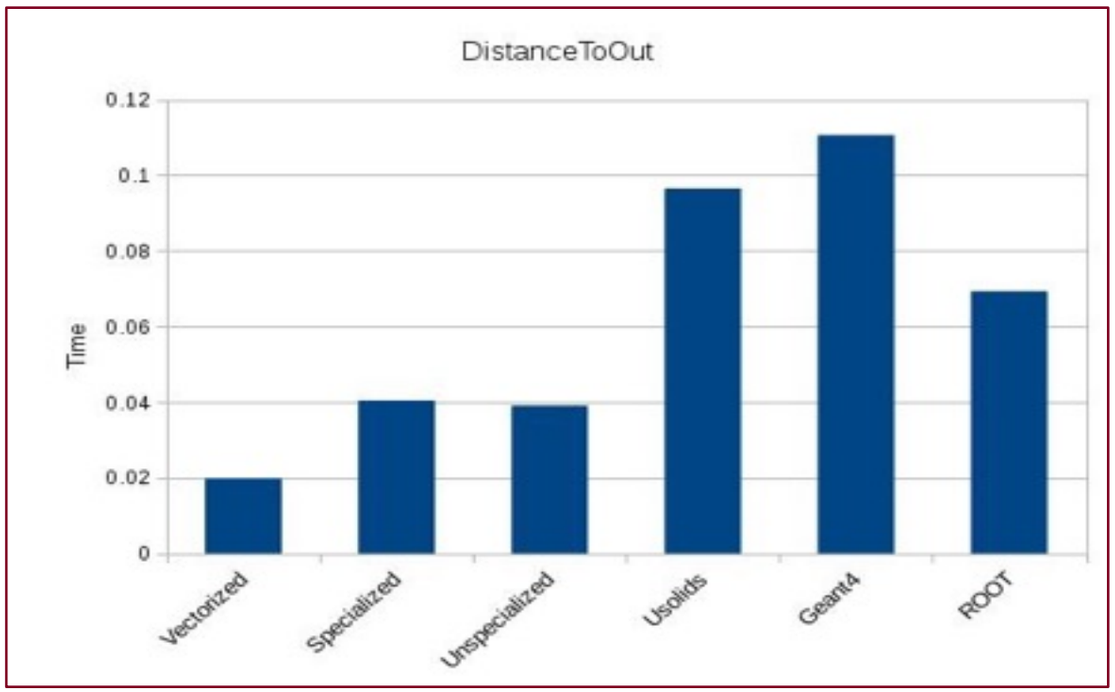
GEANTV GEOMETRY & USOLID

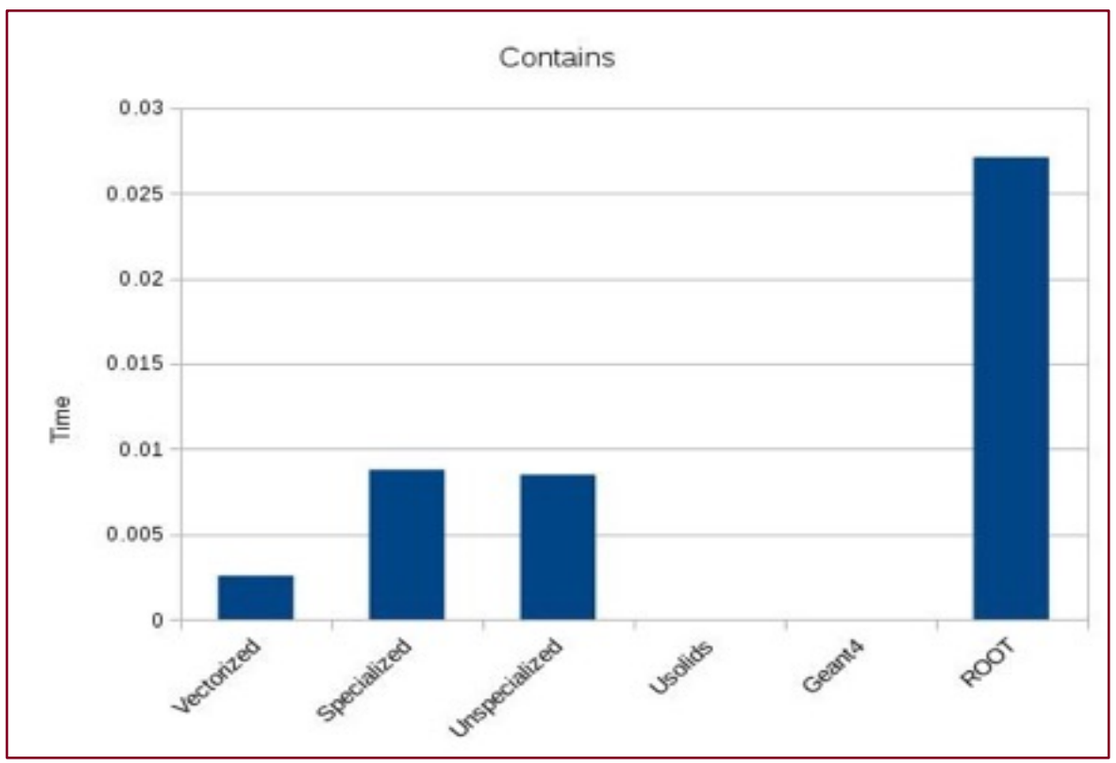
- Provide functional navigation in CMS2015 (G.Cosmo, A.Gheata, S.Wenzel, Y.Zhang)
  - Done and validated (steb-by-step)
- Refactoring, optimisation, memory reduction, I/O for Xeon Phi (S.Wenzel)
- Develop optimised voxelisation (R.Brun, G.Cosmo, S.Wenzel)
  - Different voxelisation strategies implemented and benchmarked
  - Static analysis choice of “best strategy”
- VecGeom primitive solids (A.Bhattacharyya, G.Cosmo, M.Gheata, T.Nikitina, R.Sehgal, S.Wenzel, FNAL)
  - Implemented most solids & extensive work on validation and “convention checkers”
- Simple visualisation with threejs (A.Gheata, I.Goulas, S.Wenzel)
  - First version completed

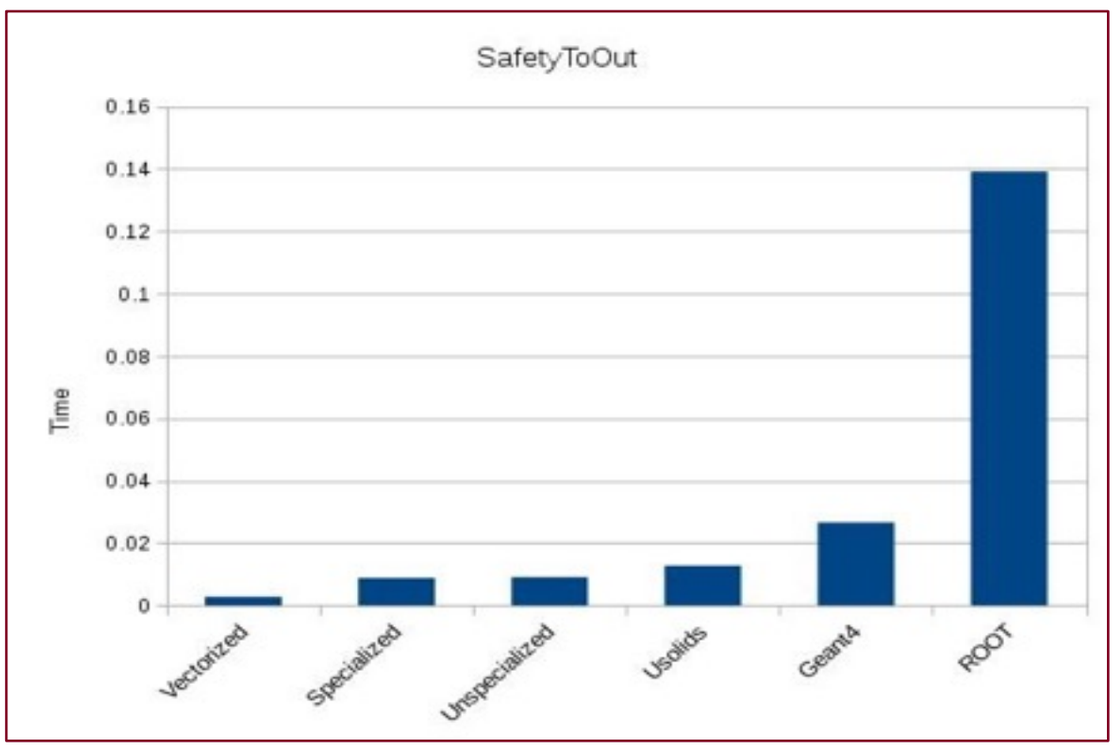


BENCHMARK RESULTS FOR CONE COMPARED TO EXISTING LIBRARIES







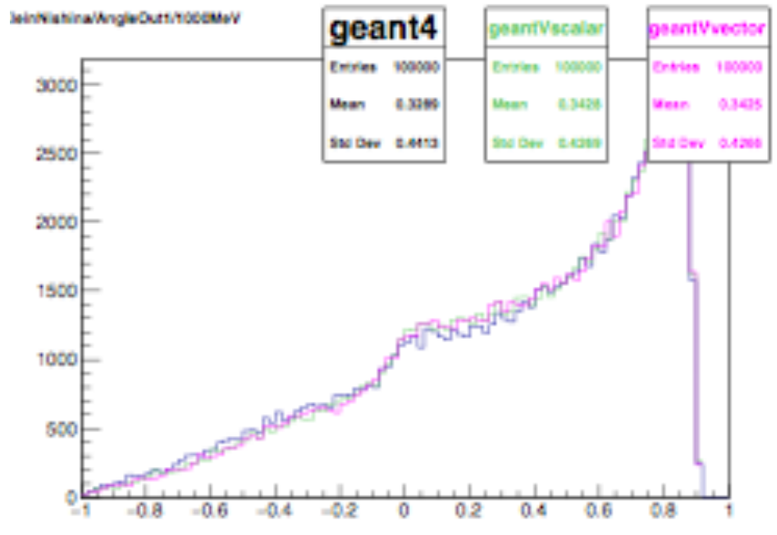


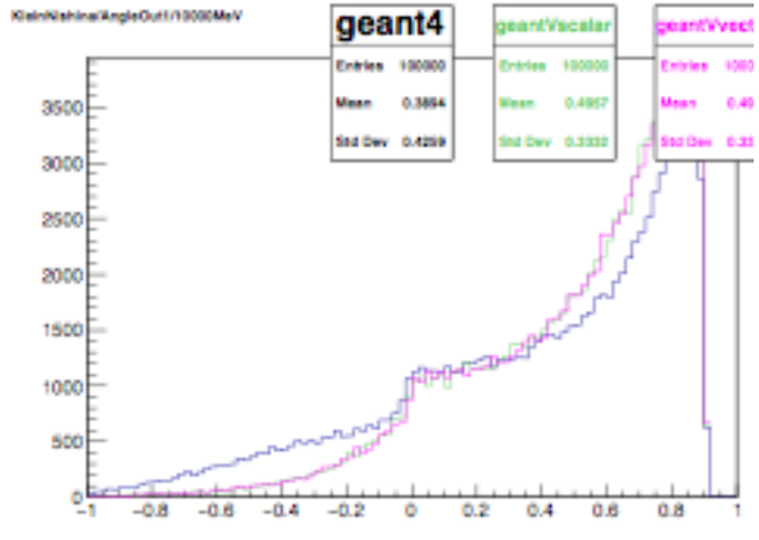
GEANTV PHYSICS

- Develop vectorised bremsstrahlung, energy loss and ionisation models (J.Apostolakis, M.Bandieramonte, FNAL, M.Novak)
  - Vectorised version of G4 code implemented and validated
  - “Alias sampling” implemented and studied, developed alternative approaches
- Vectorised version of multiple / elastic scattering (V.Ivantchenko, M.Novak)
  - Postponed to 2016
- Maintain tabulated physics (F.Carminati, M.Novak)
  - Code moved to Geant4 10 and improved
- Vectorised Runge Kutta in EM field (J.Apostolakis)
  - Scalar version ready and tested but not yet vectorised

SOME PHYSICS BENCHMARKS

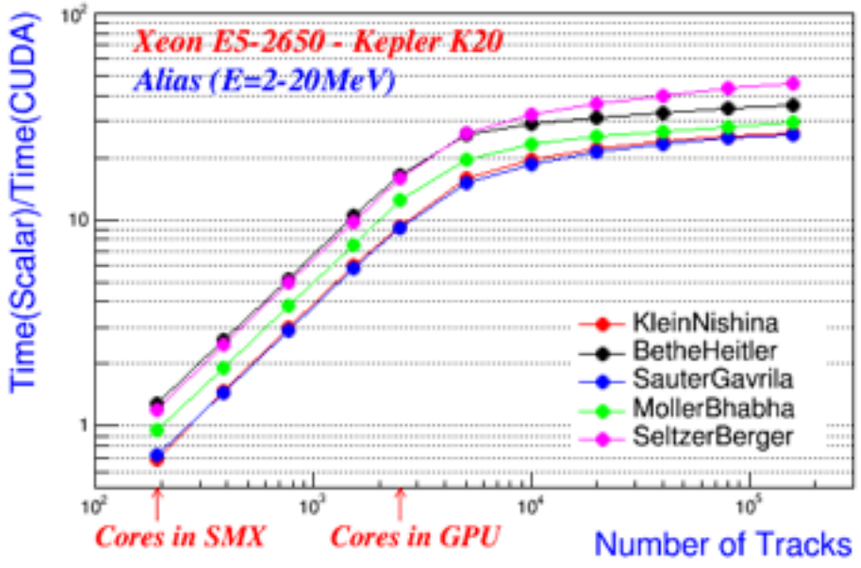
- Validation of Klein-Nishina Compton implementation



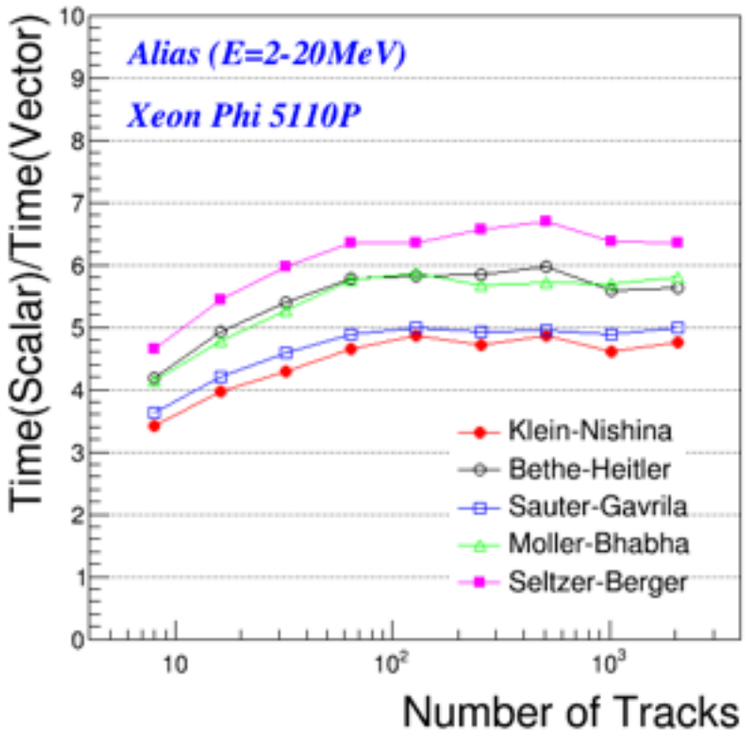


- Vector speedup of Alias method implementations of e-/g processes

1GeV



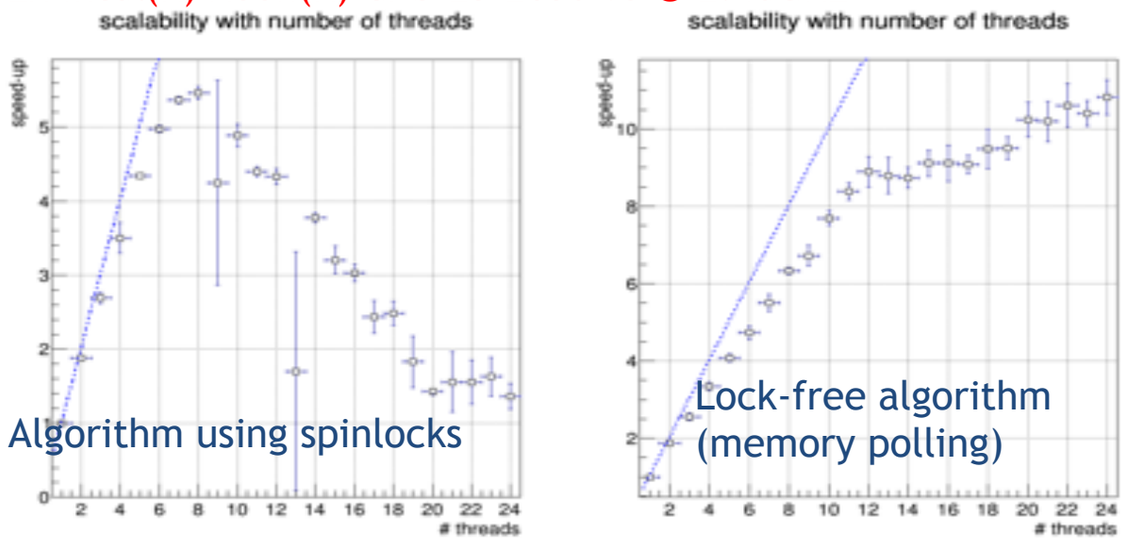
10GeV

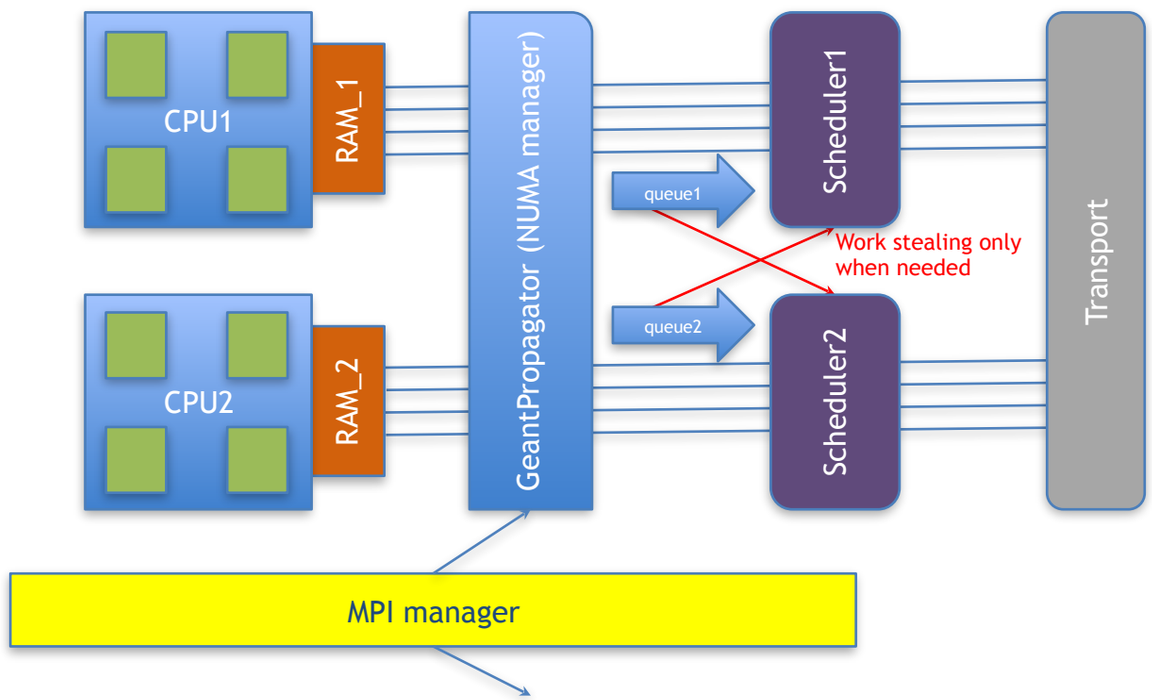


BASKETIZER PERFORMANCE AND IMPROVEMENT PLANS

- Investigated different ways of scheduling & sharing work - lock free queues, ..
- Sequential fraction still large, due to high re-basketizing load (concurrent copying)
  - O(10^5) baskets/second on Intel Core i7™
  - Algorithm already lock free
  - Rate will go down with physics processes
- Milestones 2016 to improve scalability
  - Re-use baskets in the same thread after step if enough particles doing physics-limited steps
  - Use AOS re-basketizing converted to SOA for transport
  - Clone scheduling in NUMA aware groups, important for many cores (e.g. KNL)

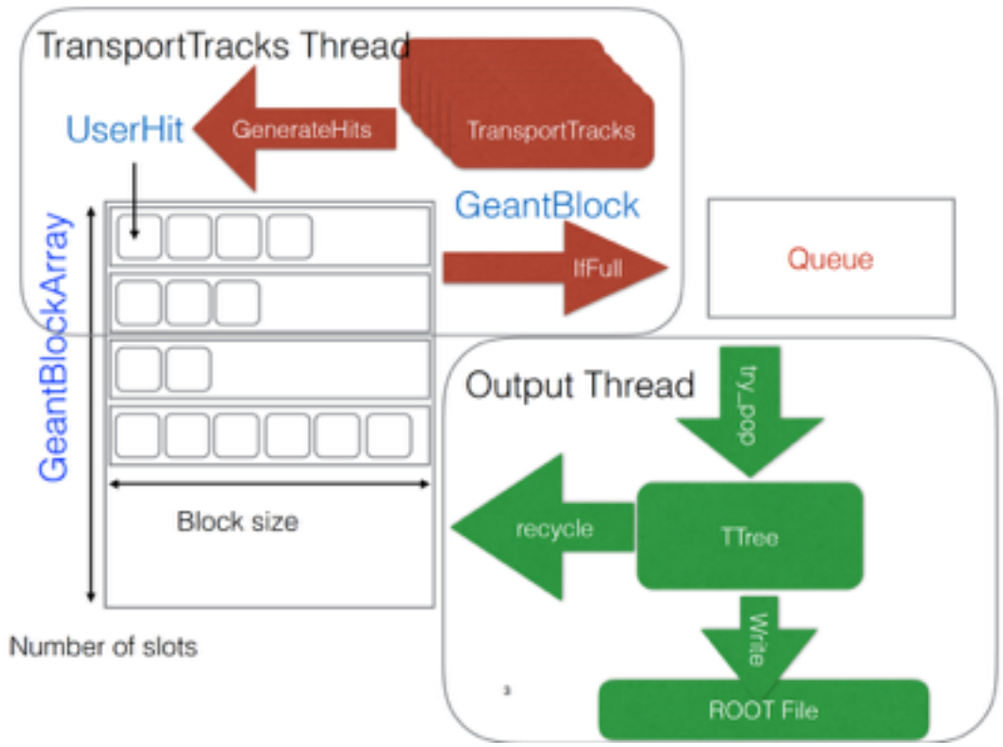
Rebasketizing
2x Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40GHz

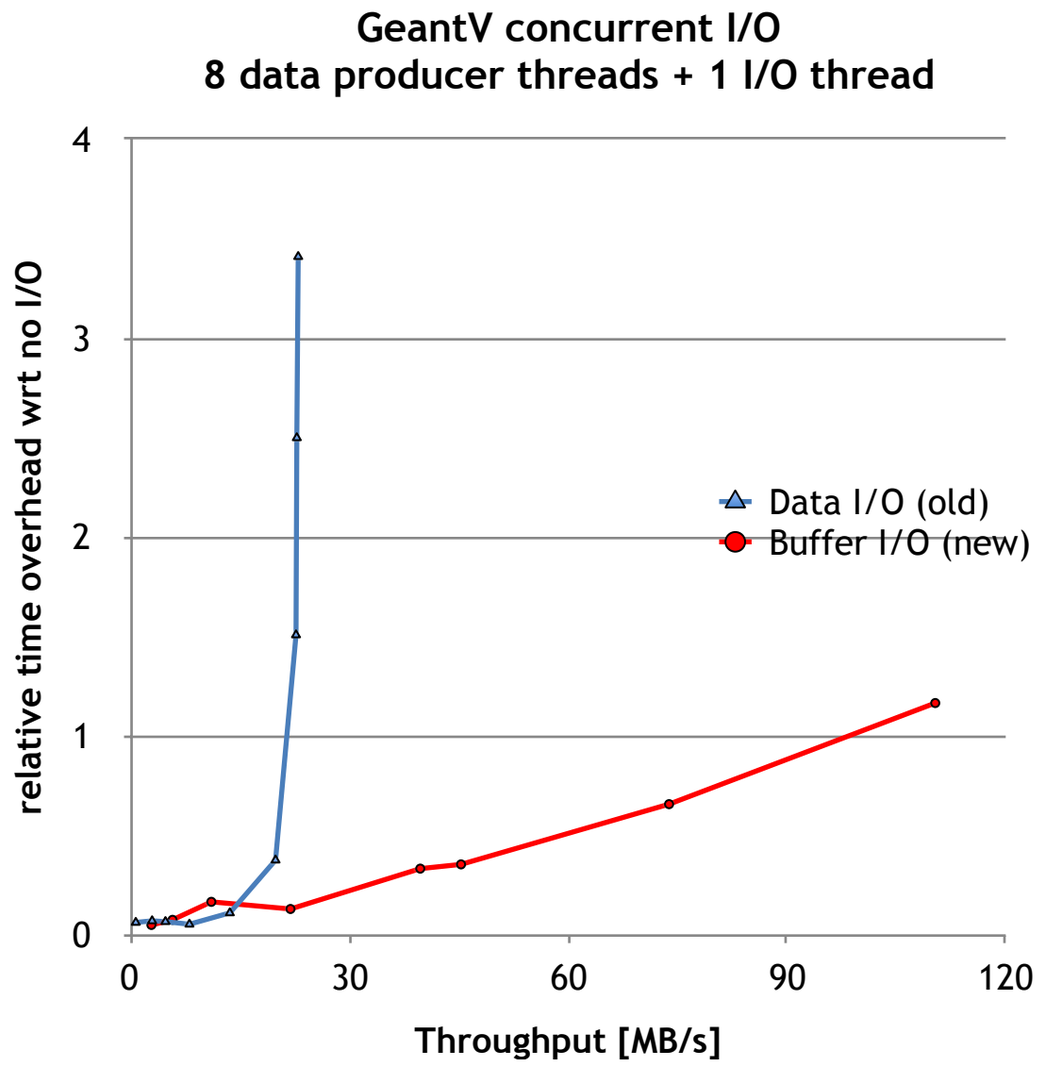




RESULTS: HITS/DIGITS I/O

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





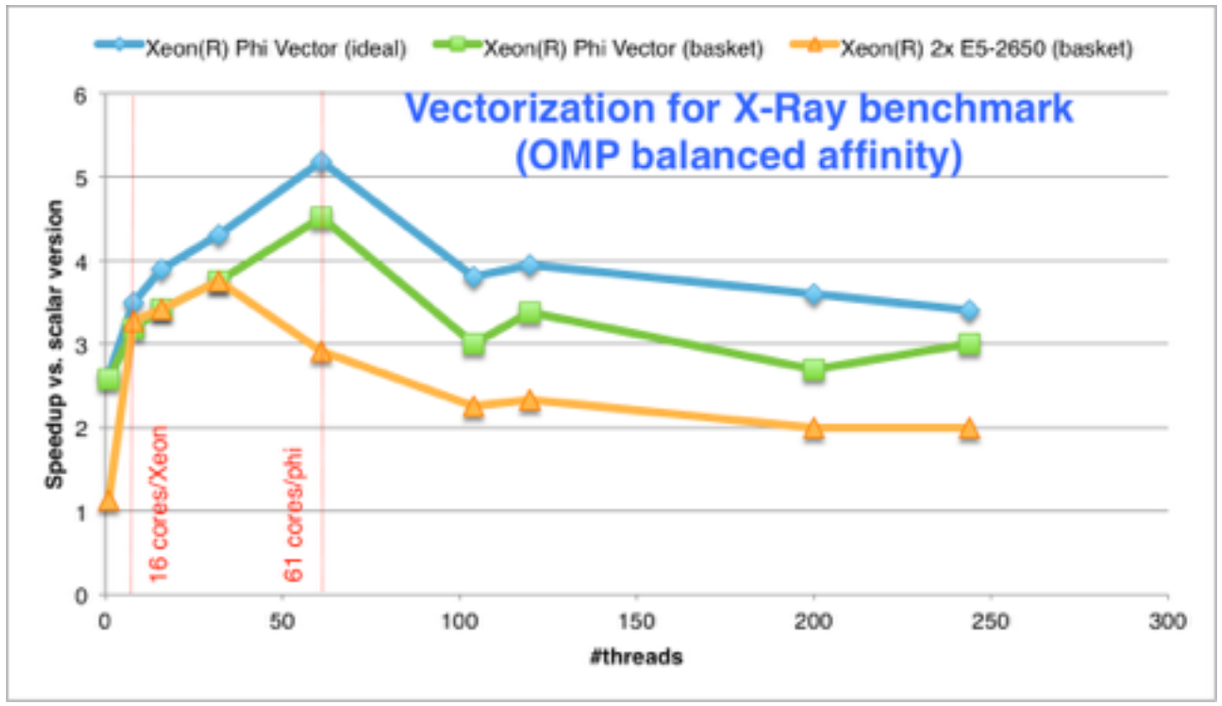
- "Buffer" mode
  - Send concurrently memory files produced by workers to one thread dealing with merging/write to disk

2x8 Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40GHz
Samsung SSD 850 PRO 512GB

VECTOR PERFORMANCE – X-RAY BENCHMARK

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

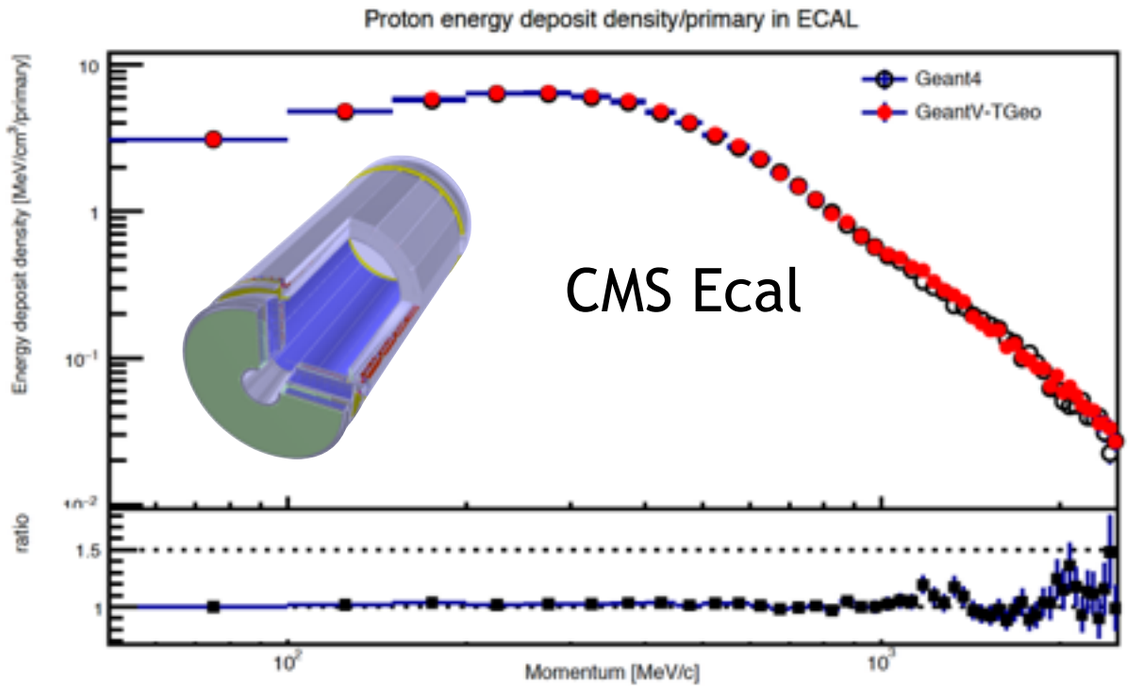
Set of concentric tubes



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

FULL SCALE DEMONSTRATOR

- Current prototype able to run an exercise at the scale of an LHC experiment (CMS)
  - Simplified (tabulated) physics but full geometry, RK propagator in field
  - Very preliminary results needing validation, but hinting already to performance improvements of factors in scalar mode

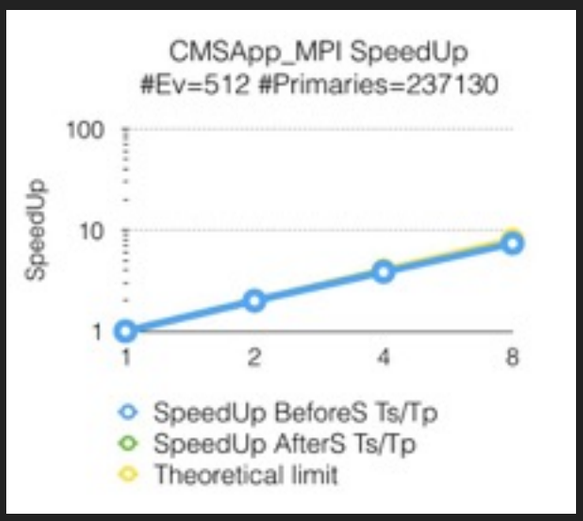


OTHER ACHIEVEMENTS

- Revise GeantV system design (all+A.Ribon, M.Novak)
  - Major design work on new classes and structures completed
- Development of ROOT-independent physics classes (F.Carminati)
- Porting and benchmarking of code to Xeon Phi (S.Vallecorsa)
- Porting of code to CUDA (S.Vallecorsa, FNAL)
- Presentation at CHEP and Supercomputing 2015 (A.Gheata)
- Build & test infrastructure on Jenkins (G.Folger, O.Shadura, P.Mendez Lorenzo)
  - All platforms including GPUs and coprocessors, support of Doxygen information publishing, nightly Coverity checks, gitlab integration

OTHER ACHIEVEMENTS

- Coding convention tools (O.Shadura)
  - Integration in jenkins of latest rules from Eclair for VecGeom & GeantV
  - Clang-format code beautification & analysis: hooks, test & documentation
- Performance tuning and monitoring (A.Gheata, O.Shadura PhD)
  - Genetic optimisation of parameters with NSGA-II algorithm with crowding distance and non-domination sorting operators
  - Ongoing work on parallel processing and concurrency of framework
  - Testing of set of DTLZx multi-objective functional evaluation with performance counters
- MPI version of the GeantV running several parallel multithreaded kernels (M.Bandieramonte)



POW 16

GEANT4 PHYSICS

- Continuous tasks (no deadline)
  - Coordination of Hadronic Working Group (A.Ribon)
  - Coordination of Electromagnetic Physics (V.Ivantchenko)
  - Maintenance of physics lists (G.Folger - coord, A.Ribon)
  - Maintenance of FTF code (A.Ribon)
  - Hadronic showers testing (A.Ribon)
  - Grid testing, reproducibility (W.Pokorski, A.Ribon)
  - Maintenance of Binary Cascade (G.Folger)
  - Representation of Geant4 in the CERN Medical Application Committee (J.Apostolakis)

CERN EXPERIMENT SUPPORT

- Ongoing tasks
- ALICE (A.Ribon)
- ATLAS (J.Apostolakis)
- CALICE (A.Ribon)
- CMS (V.Ivantchenko, G.Cosmo)
- FCC (A.Ribon)
- LHCb (W.Pokorski)

GEANT4 ELECTROMAGNETIC PHYSICS

- Investigate the Mott correction for the Goudsmit-Saunderson MS (M.Novak, V.Invantchenko)
  - 3Q16
- Development of single scattering model for e-/e+ based on Dirac PWA (best possible in 1keV-100MeV kin) (M.Novak, V.Invantchenko)
  - 1H16
- Doc & publication (M.Novak, V.Invantchenko)
  - 2H16
- Improved calorimeter response – tuning fluctuation and MS (V.Ivantchenko, M.Novak, L.Urban)
  - 2H16
- Migration of Fermi BU, General evaporation model to the common nuclear level database (V.Ivantchenko)
  - 1H16
- Specific experiment issues (V.Ivantchenko, J.Apostolakis, W.Pokorski, A.Ribon, A.Bagulya, V.Grichine)
  - ATLAS shower shape and tilecal, CMS testbeam review, ALICE move to Geant4 – PhysList, TRD

GEANT4 HADRONIC PHYSICS

- Tuning of parameters of de-excitation/pre-compound modes (V.Ivantchenko and J.M.Quesada)
  - 2H16
- Improvement of the charge exchange model (V.Ivantchenko)
  - 1H15
- Continue the maintenance of FTS & QGS codes (A.Ribon with V.Uzhinskii)
  - 1H16
- Continue the maintenance Binary Cascade (G.Folger)
  - Ongoing
- High energy models for LHC and FCC applications (V.Ivantchenko, A.Ribon and A.Bagulya)
  - 2H16

GEANT4 GEOMETRY

- Review and improvement of safety calculation in MT (J.Apostolakis, G.Cosmo)
  - 1H16
- Parallel Navigation - performance / robustness (J.Apostolakis, G.Cosmo)
  - 3Q16
- Implement use of C++11/14 constructs in the Geant4 geometry modeler (G.Cosmo)
  - 1H16
- Complete the replacement of Usolid shapes with VecGeom ones and test them with Geant4 and ALICE VMC (G.Cosmo, T.Nikitina, M.Gheta, R.Seghal)
  - 2H16 (also a GeantV item)
- Coordination geometry in Geant4 (G.Cosmo)
  - Ongoing

ONGOING PROJECTS

- Grid tests of Geant4 (D.Konstantinov, V.Pokosrski, A.Ribon)
- Support for GDML, ROOT I/O (W.Pokorski, G.Cosmo)
- Geant4&V and VecGeom POW monitoring (G.Cosmo)
- Nightly & continuous testing (G.Cosmo, G.Folger)
- Release coordination, building & installing (G.Cosmo, G.Folger)
- Coordination of the Geant4 C++11 task-force (G.Cosmo)
- Web master (G.Cosmo, G.Folger)
  - Migration to Drupal 2H16
- Coordination of GENSER (W.Pokorski, D.Konstantinov)
- Coordination of HepMC3 development (W.Pokorski, D.Konstantinov)
  - First production release 1H16
- Validation DB development (W.Pokorski, A.Ribon, FNAL, D.Konstantinov)

GEANTV OVERVIEW

- The objective of GeantV for 2016 are
  - A vector version of the most important EM processes
  - Tabulated physics for hadronic
  - A vector version of magnetic field stepper
  - Implement full vector navigator for geometry
  - Port & optimise the code to Intel Xeon Phi KNL
  - Complete porting & optimise the code on NVIDIA GPUs
  - Integrate hits parallel I/O
  - Develop kinematic and truth I/O
  - Run with at least 2 large detectors (CMS and ALICE, LHCb could be added, ATLAS has to be evaluated)
  - Continuously monitor performance with respect to Geant4

GEANTV PHYSICS

- Integration & vectorization of the new Goudsmit-Saunderson multiple scattering model (M.Novak, F.Hariri)
  - 1H16
- Integration of physics utilities (e.g. stepper, physics list, etc.) (J.Apostolakis, M.Novak, A. Ribon, F.Hariri)
  - 1H16
- Integration & validation of important EM processes (J.Apostolakis, M.Novak, A. Ribon, F.Hariri, FNAL)
  - 3Q16
- Implement realistic physics cuts and validate physics performance
  - 1Q16

GEANTV GEOMETRY & TRACKING

- Integration of the full vector navigator with physics and geometry (A.Gheata)
  - 1Q16
- Vectorization of magnetic field stepper (Ananya, J.Apostolakis, A.Gheata, FNAL)
  - 1Q16
- MonteCarlo truth and kinematic structure, with persistency (W.Pokorski, A.Gheata)
  - 1H16
- Development of I/O (hits & MC truth) for the MPI version (M.Bandiermonte, A.Gheata)
  - 1H16
- Further development of the TreeJS interface (I.Goulas)
  - Ongoing
- Developments of VecGeom & TGeo interface for VMC (AIDA-2020/WP3) (M.Gheata, G.Cosmo, FNAL)
  - 2H16

GEANTV INFRASTRUCTURE

- Demonstrate gains on accelerators with vector navigation & automatic selection of voxelisation (A.Gheata, S.Vallecorsa, FNAL)
  - 1Q16
- Documentation (J.Apostolakis, M.Novak, A. Ribon, F.Hariri)
  - 2H16
- Complete porting of tabulated physics on GPU and Xeon Phi KNC (S.Vallecorsa, FNAL)
  - 1Q16
- Detailed performance evaluation on Intel Xeon Phi (KNC) (S.Vallecorsa)
  - 1Q16

GEANTV INFRASTRUCTURE

- Port GeantV to the Intel Xeon Phi KNL (or the emulator) and evaluate performance (S.Vallecorsa, A.Gheata)
  - 1H16
- Performance analysis and optimisation on Xeon Phi KNL (S.Vallecorsa)
  - 3Q16
- Develop a fast simulation infrastructure and implement simple fast simulation algorithms from Geant4 geared toward FCC (A.Ribon)
  - 1H16
- Definition of libraries: separation between utilities, API, scheduling , I/O libraries (all, FNAL)
  - 1H16

PERFORMANCE OPTIMISATION

- Performance monitoring and tuning on all architectures (FNAL, O.Shadura, S.Vallecorsa, A.Gheata)
  - 2H16
- Genetic algorithm optimisation (O.Shadura)
  - Implementation & test of genetic operators (NSGA-III, MOAE/D-PBI, MOAE/DE)
  - Integration of MVA to reduce dimensionality
  - Production runs and evaluation of results and recommendations

CONCLUSIONS

- Just run out of steam…