Summary of Simulation Sessions

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The tools: Geant4

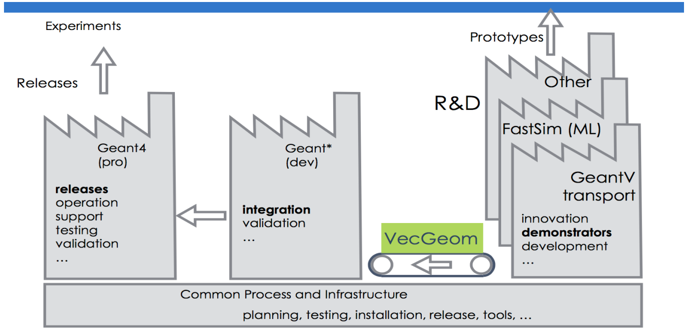
- Improve and extend functionalities while keeping user's interfaces as stable as possible
- Activities to improve physics and computing performance
  - Revise production threshold mechanism
  - Improve handling of less common particles: Ions, muonic atoms, radicals, etc
  - Refactor transportation, i.e. different for charge particles, neutrals, optical photons
  - Sub-event level parallelism: from event-level to track-level threads
- Geant4 encourages and supports various event biasing functionalities
- R&D external to G4 are of interest of the simulation community
  - Physics models, data libraries, interfaces to CAD systems
  - GeantV transport engine, track-level transport,
  - Machine learning

The tools: GeantV transport engine

GeantV R&D explores vectorized particle transport, exploiting SIMD and data locality (thread processes a basket of tracks with mixed events) – aims to 2-5 speedup factor

- Alpha tag – experiments, power users encouraged to test, provide feedback
  - Components: transportation of baskets of tracks from mixed events, vectorized geometry and magnetic field, scalar physics (full set of EM physics models), user interfaces
  - Examples: simple EM applications, standalone CMS, standalone LHCb, cmsToyGV
  - Plan for 2018 towards beta tag in early 2019
    - EM Physics fully vectorized, optimization, improved interfaces and features
    - Demonstrate speedup in a realistic application
- R&D team produces GeantV transport engine
  - If successful, the path would be integration to Geant4 toolkit for further validation, testing, support

    (VecGeom successful example)



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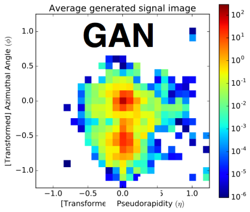
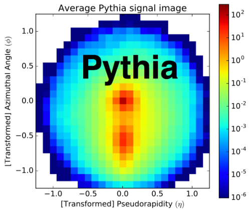
The physics: EM, hadronic, Deep Learning techniques

- Theoretical review of models for precision and extension to higher energies and to processes needed by future experiments
  - Improvement to EM physics already: multiple scattering, improved pair production model
  - Plans for further improvements: theory-based fluctuation model and NLO corrections (EM), extension of string models to high energy, refinement of low energy nuclear physics (HAD)
- Revision of algorithms for improved computing performance and vectorization
  - EM vectorization in the context of GeantV
  - Modularization and code revision of Bertini Cascade model GXBert:
    - Already a 13-25% speedup, vectorization to follow
- Machine learning to replace simulation steps
  - Started with calorimeter showers, in particular jet images using (GAN)
    - Exploit factorization of energy depositions
  - Implementation in experiments is a challenge
    - A lot of investment in R&D





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The experiments

- ATLAS following a number of strategies to speed up simulation
  - Solids improvements (4%), big library (10%), profile guided optimization
  - Geant4MT is working in Athena
  - Ideas that would change physics to be considered carefully
    - Fast calorimeter simulation, fast chain option
- CMS adopted biasing methods, testing R&D products
  - Russian roulette gave 30-50% gain, will test variable tracking parameter values (10%)
  - Co-development model: tested and adopted VecGeom with G4 10.4 for production < 2 months after release. VecGeom (scalar mode) gave 7-13% speedup
  - Successfully integrated GeantV alpha tag in toy framework (CmsToyGV)
    - Goal is verify compatibility of multithread model, test user interfaces, provide feedback
- Muon g-2 adopted VecGeom, Mu2e will consider adoption after G4 10.4 migration
- Neutrino experiments exploring LArSoft vectorization for LAr TPC simulation
  - Re-implemented small function around using VecCor (3x improvement in exec. time)

The experiments

- LHCb: extensive development to meet the challenges of Run 3
  - Exploring fast simulation options: parametric approaches, frozen showers and machine learning
    - Aim to speed up calorimeter simulation by factor of 3-10
  - Re-write of simulation framework (Gauss) to benefit from improvements to Gaudi and G4
    - Will allow best mix of simulation options for different physics analyses
- ALICE undergoing major changes in software stack to cope with Run3/4 challenges
  - Dedicated optimization program leveraging data monitoring and tools, heterogeneous architecture targeting track-level paralelism,VecGeom navigation to replace TGeo, integrated full and fast simulation framework, improved workflow on grid
  - Support R&D, e.g. the GeantV engine, explore future integration
- The path forward of G4 applications on HPC
  - Multi-process, multithreaded parallelism, MPI -done, distribute code efficiently -done, containers for workload deployment -done, leverage accelerators -under study
    - Hybrid machines remain a concern with respect to how to use accelerators efficiently
      - Only highly specialized workloads have shown promising results

Outlook

- Vigorous and diverse R&D program underway along the lines established in the CWP Roadmap
  - Improvements to toolkits, physics,
  - Machine learning applications
  - HPC porting, testing

- Work is performed within the experiments or in community organized R&D teams

- Community sponsored events have proved to be a very efficient channel for continuous improvement in communication between different R&D teams, between the experiments, and between R&D teams and the experiments