Fermilab U.S. DEPARTMENT OF ENERGY Office of Science

Simulation Directions

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Computing R&D Micro-Retreat

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Directions by the Community

- Geant4: multi-threading capable since 10.0 – event level parallelism
  - Sub-event (particle) level multithreading (Grid, Cloud, HPC systems)
  - Revise production threshold and refactor transportation (by particle type)
- GeantV: alpha version available (vectorized geometry, scalar EM)
  - Fine-grain track level parallelism aiming for 2-5 speedup (locality+SIMD)
  - VecGeom is adopted by CMS and beta (EM vectorization) is underway
- Other R&D activities
  - Fast simulation: parameterization and Machine/Deep learning
  - Modularization: task level applications, vector libraries (VecCore)
- General strategies: Improve and extend functionalities while keeping user's interfaces as stable as possible
  - Detector Simulation CWP paper (HSF) (draft) – define a roadmap by the whole international simulation community
  - A summary talk by Daniel Elvira at Joint WLCG and HSF workshop (26-28 March, 2018, at Napoli)

Challenges: SIMD (Vectorization) and SIMT(GPU)

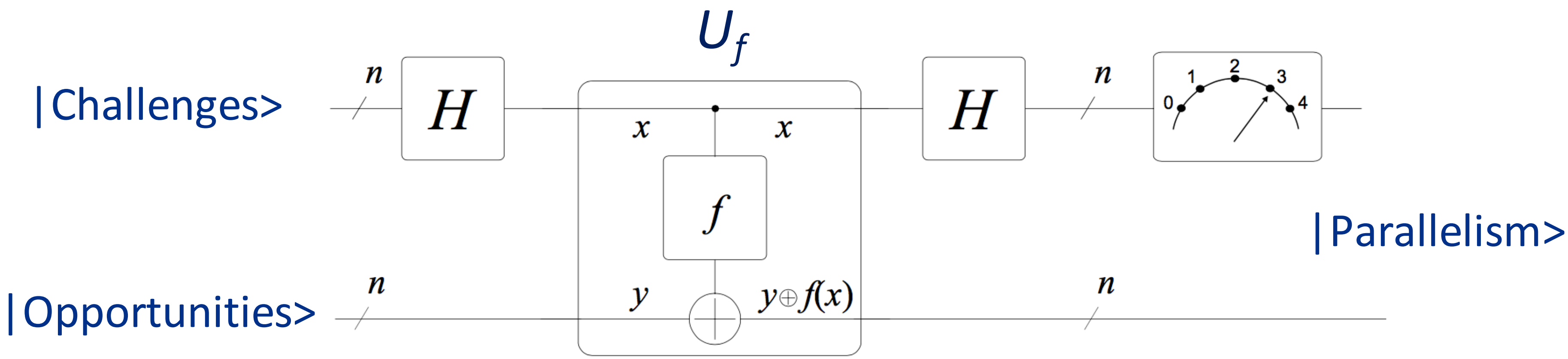
- End-to-end parallelism using SIMD/SIMT architectures is very hard for detector simulation – Hello to Amdahl
  - Path dependent simulation chains (sequential, branches)
  - Stochastic processes and final state samplings (non-deterministic)
  - Memory intensive: low FLOPS/(memory transaction)
- Vectorization (SIMD)
  - Both hardware and software are moving-targets: Ex. KNL → novel architectures and explicit SIMD instructions → c++20
  - scalability with dynamic scheduling should be proved
- Co-processors (many cores, massively many cores)
  - GPU+nvlink: off-load overhead (even for DL)
  - Target special applications (reuse-data and arithmetic intensive)
  - Ex. Neutron transport, Optical photons, EM shower, ..
- Strategies: R&D → Geant4 → support Experiments

R&D for Near-term and Far-future

- ML/Deep Learning for simulation (on-going or proposed)
  - Generative adversarial network for calorimeter simulation (CaloGAN)
  - Physics awareness ML techniques (cross sections, interactions)
- Challenges for DL supremacy in “HEP detector simulation”
  - Training by limited hyper-parameters (even with GAN) may not be good enough: ML/DL vs. parameterization (domain knowledge)
  - Explore more advanced architectures: GAN+Adversarial auto-encoder
  - Questions: large latent space and scaling on HPC systems (I/O)
- Quantum computing
  - Most models are quantum processes (ex. MSC, Compton, INCL, …)
  - However, hard to realize output (quantum superposition with coherent random processes → macroscopic collapse): a lot of qubits and hard to achieve quantum supremacy (w.r.t classical approach)
- Strategies: open to novel ideas and push boundaries

Summary: Detector Simulation R&D

- Simon's gate for Simulation R&D



  - |Parallelism> = (R&D operators) $\frac{|Challeges>+|Opportunities>}{\sqrt{2}}$
  - Covert challenges (software) and control opportunities (hardware)
  - Amplify performance gain before realization (optimization)
- Vigorous and diverse R&D program underway along the line established in the CWP roadmap and work is performed within the experiments or in community organized R&D teams (from the Daniel's summary talk)