GPU Prototype

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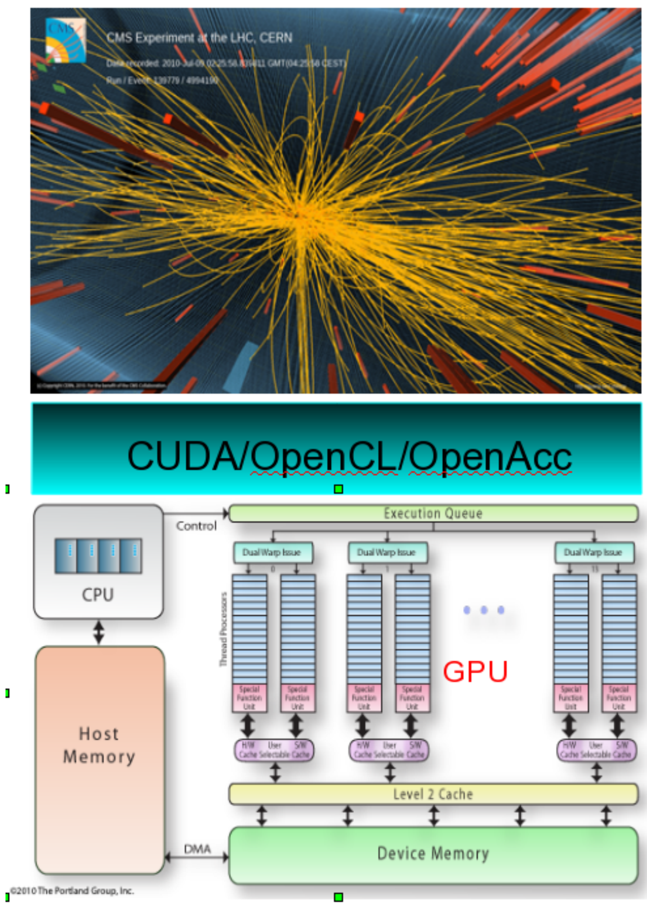
Introduction

- Future HEP software for HPC/HTC
  - hardware landscape is rapidly changing for power efficiency (advent of the many core era)
  - parallelism is no longer optional, but it must be explored thoroughly and present many challenges
  - maximize instruction throughput and data locality
- Our vision for HEP/HPC detector simulation
  - to have a massively parallelized particle (track level) transportation engine
  - comply with different architectures (GPU, MIC and etc.)
  - draw community interests for collateral efforts

Detector Simulation in GPU as a show-case

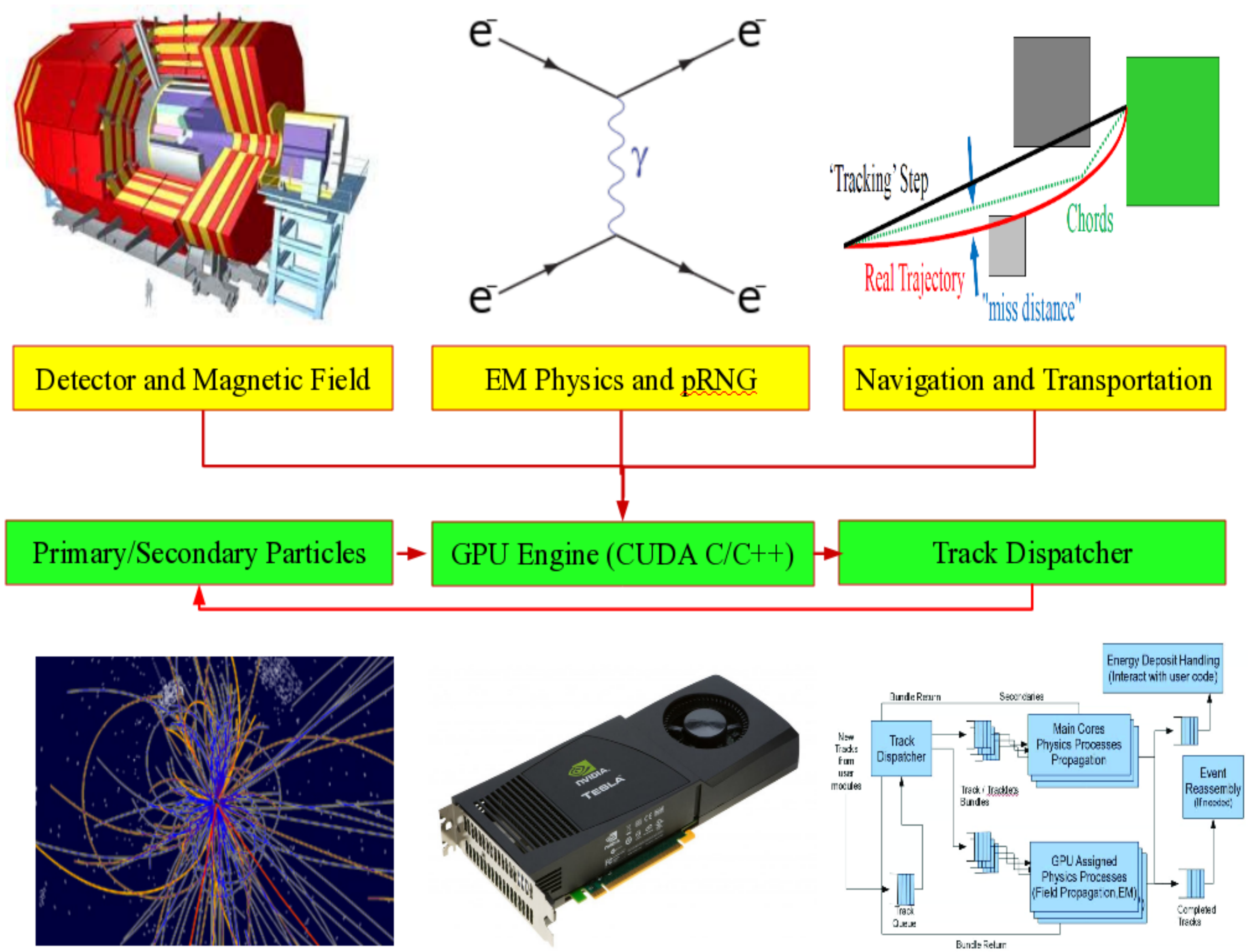


- Geant4 for detect simulation
  - highly sequential to reduce memory requirement (if-else)
  - event-level parallelism to take an advantage of using clusters
  - provided high-quality detector simulation for HEP
- GPU (CUDA) applications
  - require maximum SIMD/SIMT in conjunction with TLP
  - a good example of hybrid HPC (CPU/GPU work/load balancing)
  - many opportunities for challenging development in algorithms and efficient memory managements

Problem Statement

- Develop a massively parallelized EM particle transportation engine for many-core architects
- Key components for a (GPU) prototype
  - transportation (in a realistic magnetic field)
  - geometry (a simple detector description)
  - EM physics (electrons and photons)
  - concurrent CUDA kernels
- Consideration for GPU applications
  - reduce branches (avoid thread-level divergences)
  - reuse data (efficient memory transactions, latencies)
  - pRNG, floating-point, multiple streams and etc.

Overview of key components



Overview of GPU Kernels

- Asynchronous data transfer (tracks from a dispatcher)
- Other input data (one time allocation on global memory)
  - random states (MTwister) for each thread
  - detector geometry and a magnetic field map
  - physics tables (x-secs, brem, ionization tables, and etc.)
  - containers for secondary tracks/temporary stacks
- Stepping/tracking (split) kernels
  - GPIL-kernel
  - sorting tracks by the physics process
  - DoIt –kernel
- Also separate kernels for electrons and photons

Performance

- Hardware (host + device)

	Host (CPU)	Device (GPU)
M2090	AMD Opertron™ 6134 32 cores @ 2.4 GHz	Nvidia M2090 (Fermi) 512 cores @ 1.3 GHz
K20	Intel® Xeon® E5-2620 24 cores @ 2.0 GHz	Nvidia K20 (Kepler) 2496 cores @ 0.7GHz

- Performance measurement
  - (4096x32) tracks
  - Gain = Time(1 CPU core)/Time(total GPU cores)
    Time=(data transfer + kernel execution)
  - default <<< Block, Thread >>> organization
    M2090<<<32,128>>> and K20<<<26,198>>>

Particle Transportation

- Transport a particle for a proposed step length in a magnetic field (volume based CMS B-field map)
  - photon kernel: linear navigator
  - electron: propagation in a magnetic field
- Arithmetic intensity of the adaptive step control
  - occupancy/off-chip memory operand is low
  - data transfers between host and device >> kernel time
- A full chain of transportation requires geometry
  - geometry intersect and other decision trees
  - add intensity, but also introduce kernel divergence and memory operands (require optimization for SIMT)

Performance - Transportation

- Decompose transportation by the particle type
  - separate kernels is ~30% faster for γ:e- = 0.2:0.8 mixture
- Performance of numerical algorithms for the equation of motion of a charged particle in a magnetic field

GPU Type	Algorithm	CPU[ms]	GPU[ms]	Kernel[ms]	CPU/GPU	CPU/Kernel
M2090	Classical RK4	106.9	9.7	2.6	10.9	41.0
	RK-Felhberg	119.3	9.9	2.8	12.0	42.3
	Nystrom RK4	39.4	7.9	0.8	5.0	51.8
K20	Classical RK4	78.6	4.5	1.7	17.5	47.4
	RK Felhberg	87.9	4.4	1.6	19.8	55.2
	Nystrom RK4	30.9	3.5	0.7	8.6	46.9

Geometry

- A set of geometry classes to support EM physics and the particle transportation
  - material (element, material and Sandia table)
  - solids (box, tubs and etc.) and logical/physical vol.
  - Navigator, multilevel locator
- A simple, but realistic detector is constructed on CPU and re-mapped on GPU global memory
- Create a navigator per thread on GPU and reuse it (locating the global position is expensive)

EM Physics

- Processes and models implemented

Primary	Process	Model	Secondaries	Survivor
e^-	Bremsstrahlung	SeltzerBerger	γ	e^-
	Ionization	MollerBhabhaModel	e^-	e^-
	Multiple Scattering	UrbanMscModel95	–	e^-
γ	Compton Scattering	KleinNishinaCompton	e^-	γ
	Photo Electric Effect	PEEffectFluoModel	e^-	–
	Gamma Conversion	BetheHeitlerModel	$e^- e^+$	–

- Use look-up tables for lambda and other parameters for energy loss and sampling
- Secondary particles are stored atomically on GPU, and may be transported to CPU or rescheduled for the next tracking cycle on GPU

Global Memory

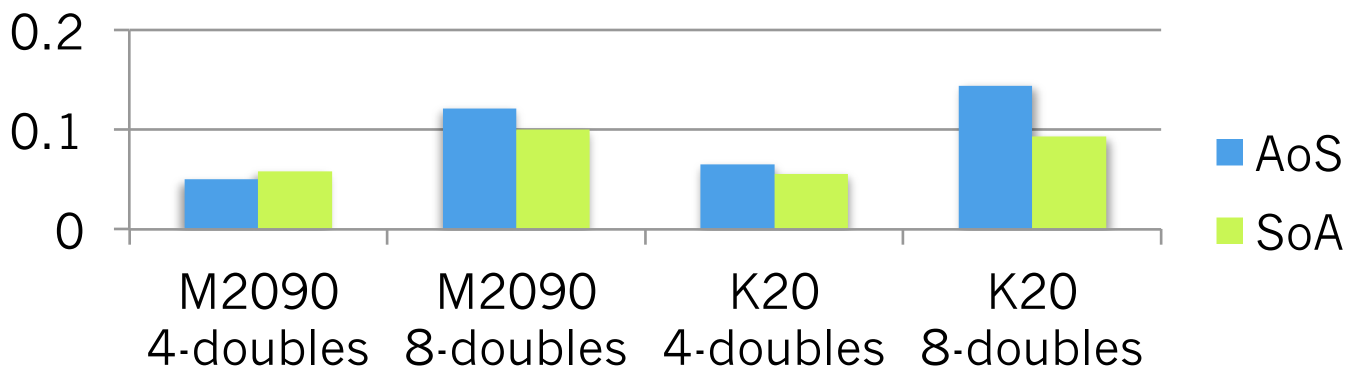
- EM physics processes and models require frequent data access from/to global memory
  - input: material information, physics tables
  - output: secondary particles (N=0,1,2 per step) and hits
- Memory transaction (atomic add) for 100K secondaries

NVIDIA M2090 <<<32,128>>>	GPU [ms]	CPU [ms]
Pre-allocated fixed memory	1.5	39.5
Dynamic allocation per thread	49.8	59.1
Dynamic allocation per block	79.0	59.0

- Strategies for secondary particles, hits and etc.
  - any dynamic memory allocation is very expensive
  - use pre-allocated memory (a fixed size stack on GPU)

Data Structure

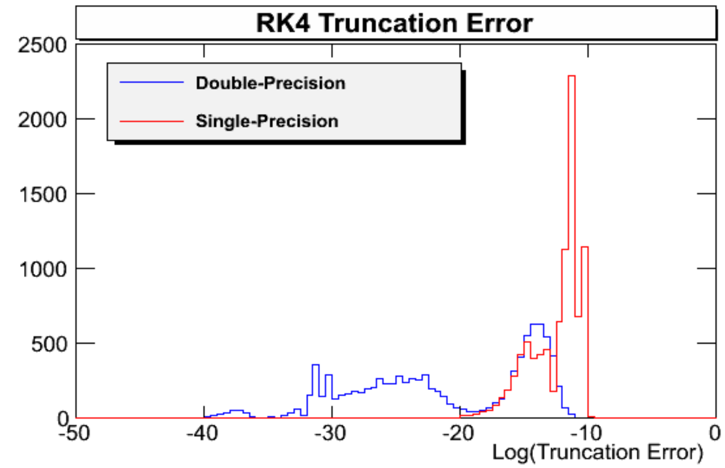
- Coalesced global memory access
  - align memory address for efficient data access
- Array of Struct (AoS) vs. Struct of Array (SoA)
  - a simple test of loading data (4-doubles, 8-doubles) and writing back to the global memory (65K accesses)

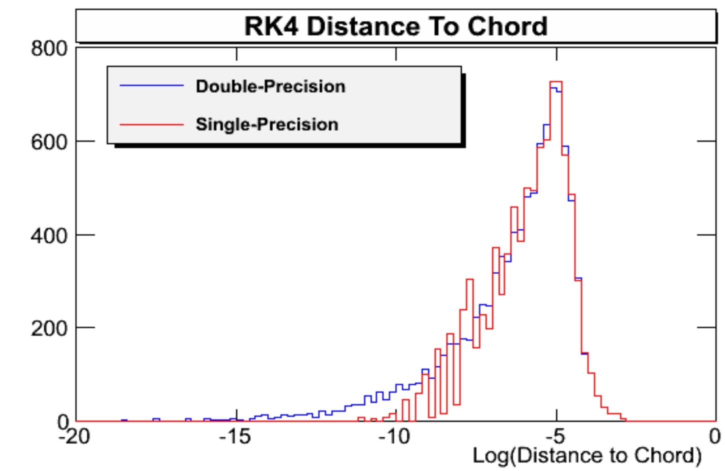


  - CPU: really depends in the size of data and architecture

Floating-point Consideration

- Cost for double-precision
  - memory throughput (x2)
  - possible registers spilling
  - cycles for arithmetic instructions (x2/x3 in M2090/K20)
  - performance in classical RK4: float/double = 2.24 (M2090)
  - not negotiable for precision and accuracy
- Possibilities for single-precision
  - input physics tables
  - B-field map (texture)
  - local coordination





Random Number Generators

- SIMD random number engine in each thread
- CUDA pRNG library (CURAND)
  - xor-family (XORWOW)
  - L'Ecuyer's multiple recursive generator (MRG32k3a)
  - Mersenne Twister (MTGP32, 32bit, period 2^11213)
- Performance: (64 blocks x 256 threads)
  - two kernels (initialize states, generation) for efficiency

CURAND pRNG	Init States [ms]	10K RNG [ms]
XORWOW	4.12	7.92
MRG32k3a	5.02	21.88
MTG32	0.69	31.94

Performance: Realistic Simulation

- A simple calorimeter (a.k.a CMS Ecal)
- Tracking for 1-step: split kernels (GPIL+sorting+DoIt)

	CPU [ms]	GPU [ms]	CPU/GPU
AMD+M2090	748	37.8 (62.6)*	19.8 (11.9)*
Intel®+K20M	571	30.4 (81.9)*	18.7 (7.0)*

()* GPU time using one kernel (sequential stepping)

- Optimization strategies
  - kernel basis (high-level restructuring)
  - component basis (low-level improvement by profilers)

Other Considerations

- Understanding performance of sub-components
  - profiled each physics process/model
  - identified divergent instructions (inefficient sampling for parallel execution, do-while, ...)
  - unit tests for algorithms and data structure
- Efficient sorting without using thrust::sort (bucket-based sorting)
- Multiple streams and concurrent kernels
- Validation
  - device codes vs. identical host codes (executed on CPU)
  - host codes vs. back-ported CPU codes

GPU Connector to an External Scheduler

- Vector Prototype (presentation by Federico) can serve as the track buckets provider to the GPU prototype
- GPU connector is an interface to the Vector Prototype
- Challenges
  - different geometry implementation – need to translate location and history information back and forth
  - difference in data layout
  - only a subset of particle can be handled
  - (ideal) bucket size very different from CPU
  - try to maximize kernel coherence

GPU Connector to the Vector Prototype

- Implementation
  - send back to CPU particles not handled
  - stage particles in a set of buckets
    - list and type of bucket is customizable, one idea is to buckets based on particle/energy that have a common (sub)set of likely to apply physics.
    - within this baskets the particles are placed in order/group given by the VP
  - delay the start of a kernel/task until it has enough data or has not received any new data in a while
  - to maximize overlap uploads are started for a task after handling a CPU basket

Future Plan

- Continue integration with the vector prototype
  - demonstrate a working example with the connector
  - share components (geometry, physics, transport and data structure)
- Redesign the prototype optimally for SIMT/SIMD
  - minimize branches (granulize tasks)
  - maximize locality (instruction and memory)
  - efficient data structure, algorithms and kernel managers for leveraging parallelism/vectorization
- Consideration for hybrid computing models
  - MIC (TBB), OpenCL and etc.