Geant4 Particle Transportation on GPU

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Concurrent Programming Models and Frameworks
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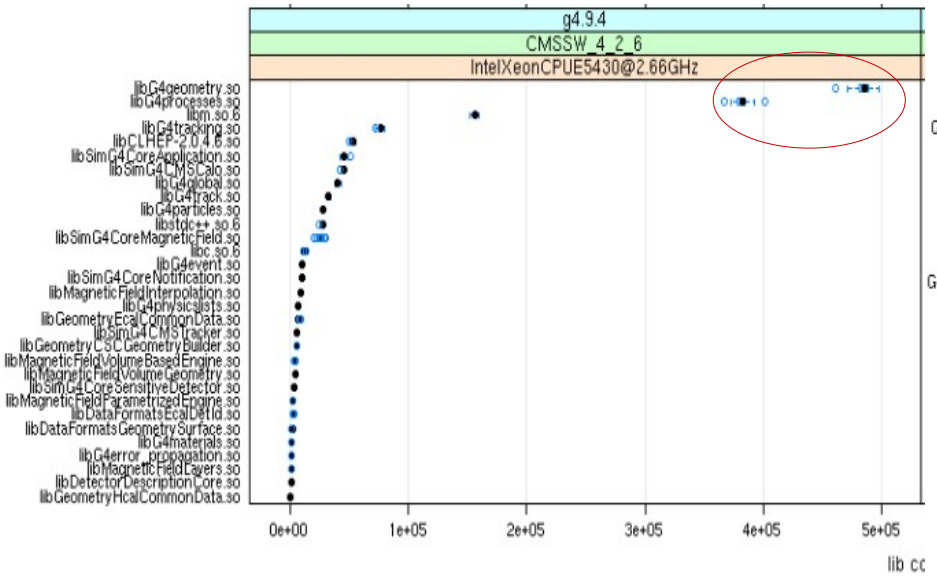
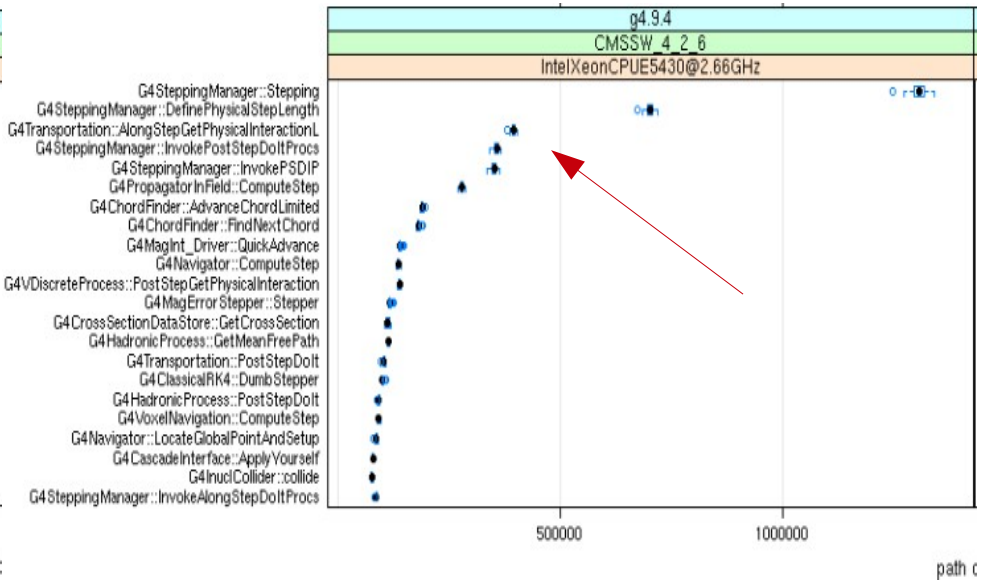
Outline

- Introduction: particle transportation
- Hardware: host and device
- Software: device codes and interfaces
- Performance: CPU/GPU processing time
- Conclusions: lessons and outlooks

Introduction

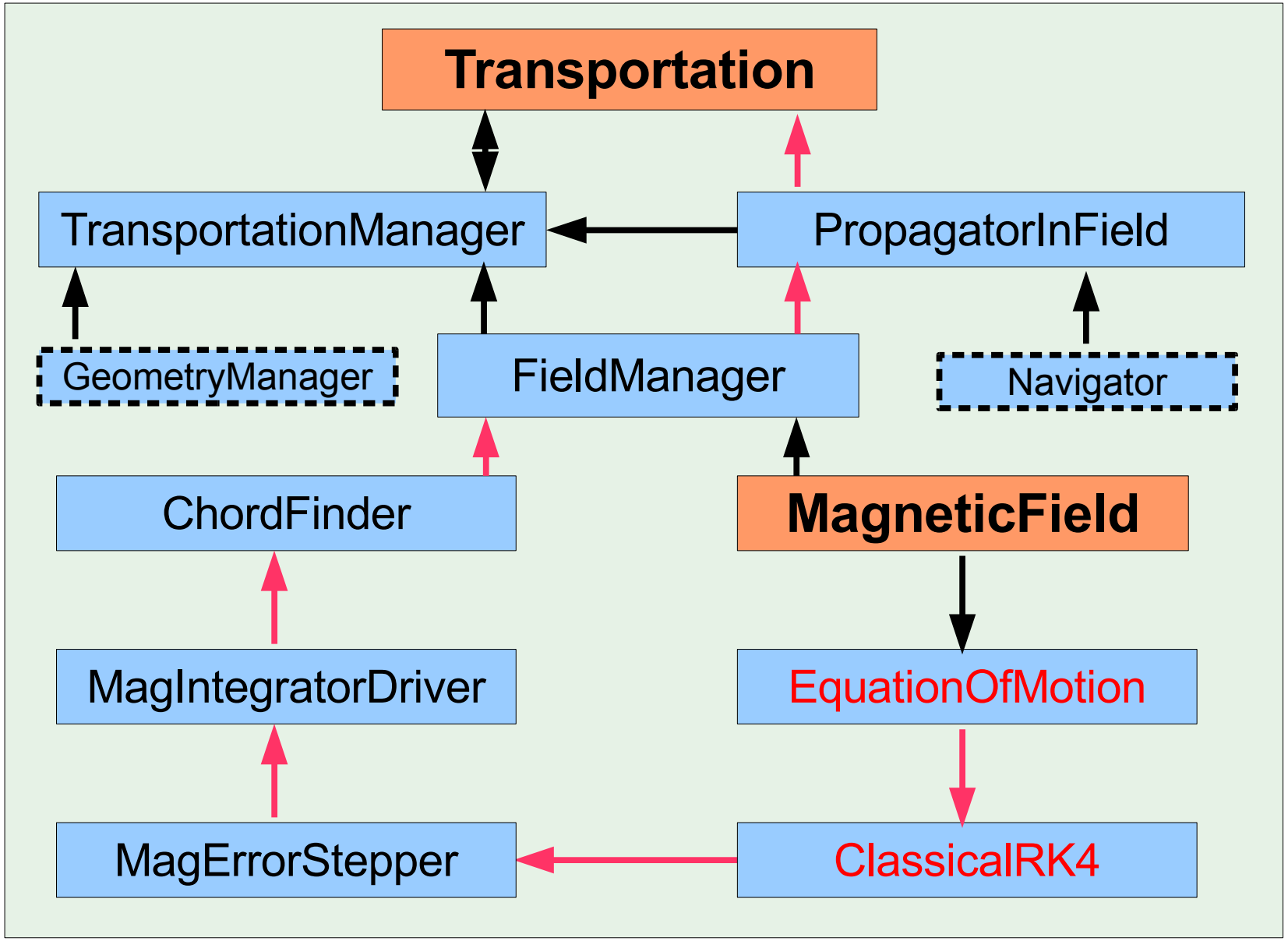
- How can we use many-core for Geant4?
- Geant4 performance studies with the CMS detector





  - geometry and processes are top libraries in lib count
  - one of hot spots of processes is transportation
- Concurrent particle transportation engine
  - study particle transportation on GPGPU

G4Transporation::AlongStepGPIL for Charged Particles in B-Field



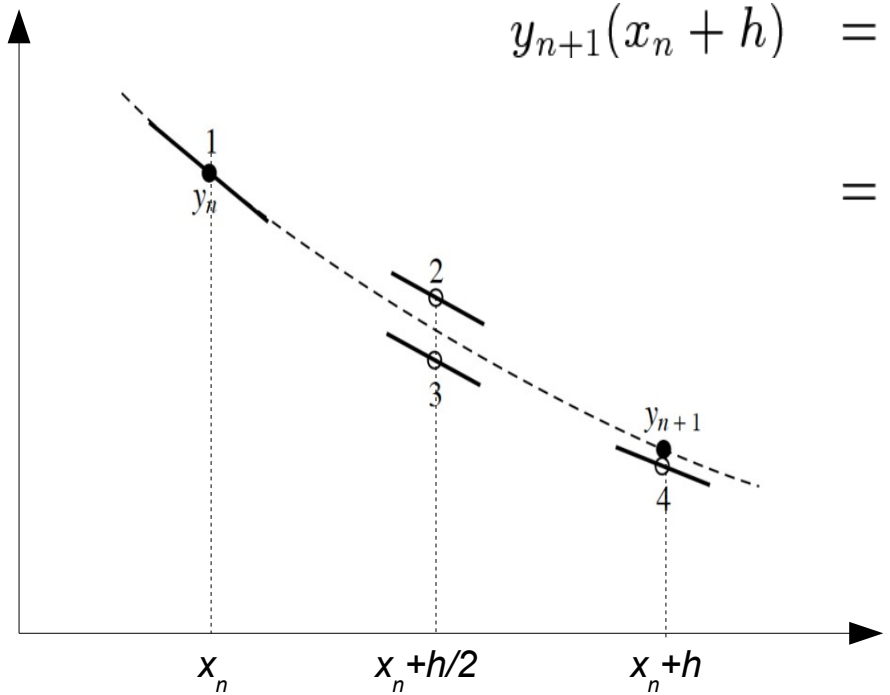
Equation of Motion and Runge-Kutta Method

- Trajectories: equation of motion in a magnetic field

$$\frac{d^2\vec{x}}{ds^2} = \frac{q}{p}\frac{d\vec{x}}{ds} \times \vec{B}(\vec{x}) \quad \rightarrow \quad \frac{dy}{ds} = f(x,y), \qquad y(x_0) = y_0$$

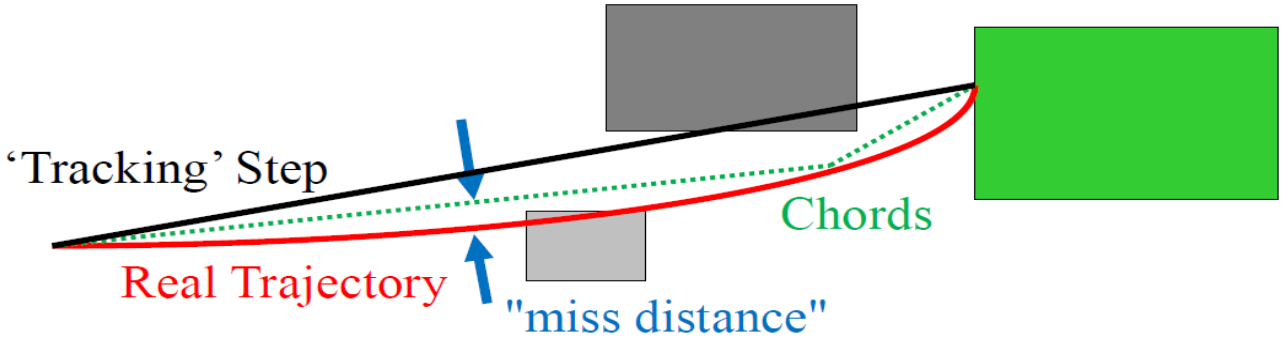
- 4-th order Runge-Kutta (RK4): 4 evaluations of f(x,y)

$$\begin{aligned} y_{n+1}(x_n + h) &= y_n + hf(x_n, y_n) \\ &= y_n + \frac{h}{6}\sum_{i=1}^{4}[f(x_n + \alpha_i, y_n + \beta_i)] + \mathcal{O}(h^5) \end{aligned}$$

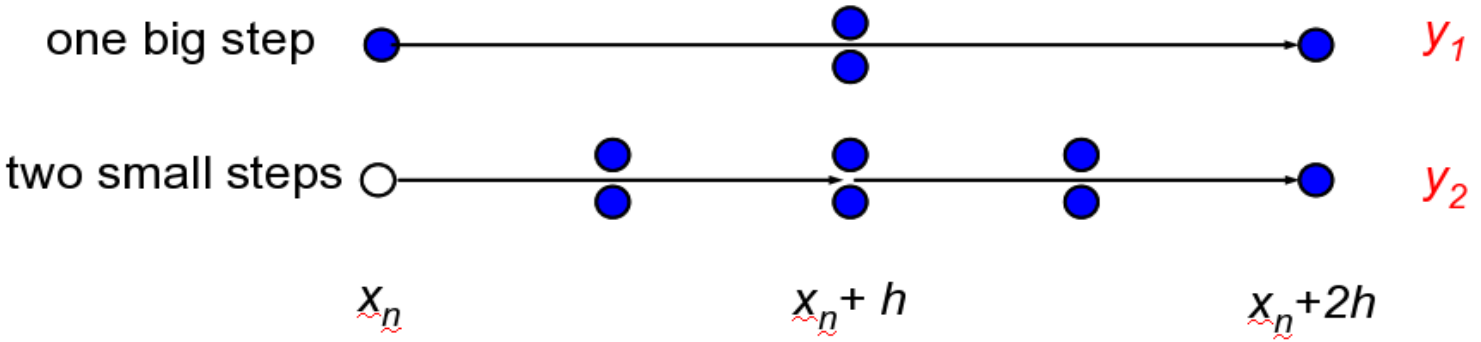


Runga-Kutta Driver with Adaptive Step Size

- Quick advance: miss distance < dmax



- Accurate advance: truncation errors of step doubling in RK4: difference between one big step and two small steps - 11 evaluations of rhs of the equation of motion



$\Delta = y_2 - y_1$ = truncation error

Problem Definition

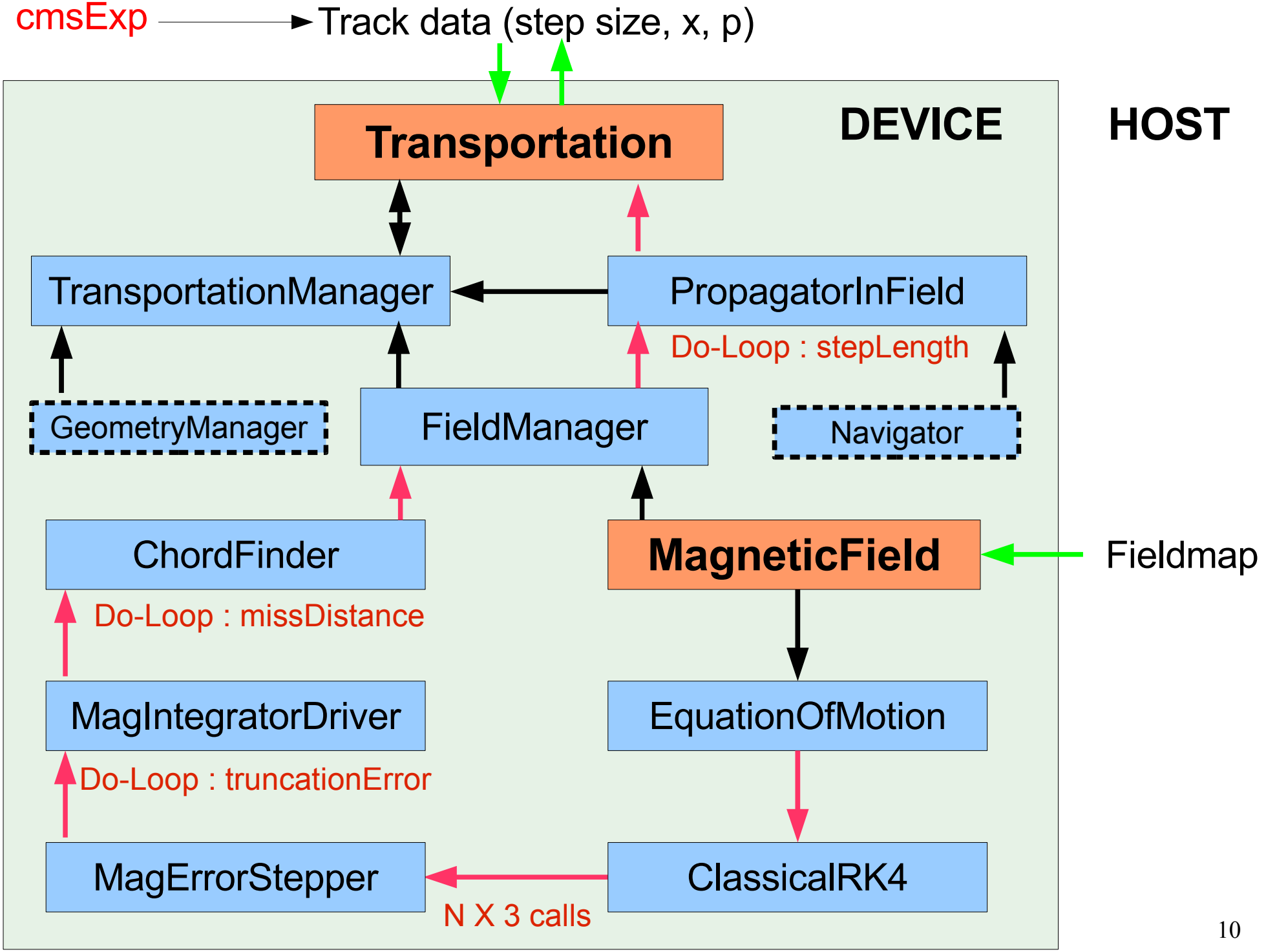
- Isolate key components of Geant4 particle transportation
  - evaluation of magnetic field (B) values
  - rhs of the equation of motion in a given B
  - evaluation of the 4^{th} order Runge-Kutta (RK4)
- Measure performance with the Runga-Kutta driver for adaptive step size control
- Test Geant4 transportation with realistic data
  - prepare bundles of tracks from simulated events
  - measure processing times for AlongStepGPIL on CPU and GPU

Hardware: Host and Device

- Host: AMD Opteron Process 6136
  - CPU: 2.4 GHz, Processors: 32 cores
  - L1/L2/L3 Cache Size: 128/512/12288 (KB)
  - L3 Cache speed: 2400 MHz
- Device: NVIDIA Tesla M2070
  - GPU clock speed: 1.15 GHz
  - 14 Multiprocessors x 32 CUDA Cores: 448 CUDA cores
  - Memory: global 5.4 GB, constant 65 KB, shared 50KB
  - L2 Cache size: 786 KB
  - Maximum thread per block: 1024
  - Warp size: 32
  - CUDA Capability Major/Minor: 2.0

Software: Interface and Device Codes

- An experimental software environment: cmsExp
  - CMS geometry (GDML) and magnetic field map (2-dim grid of volume based field extracted from CMSSW)
  - Geant4 application with an interface to device codes or a standalone framework
- Device codes I
  - literal translation of Geant4 C++ classes to C structures
  - use same implementation for both __host__ and __device__
  - input data to device memory: magnetic feld map and bundles of secondary tracks produced by cmsExp
- Device codes II optimized for GPU
  - 4^{th} order Runge-Kutta, field map with texture memory and etc.

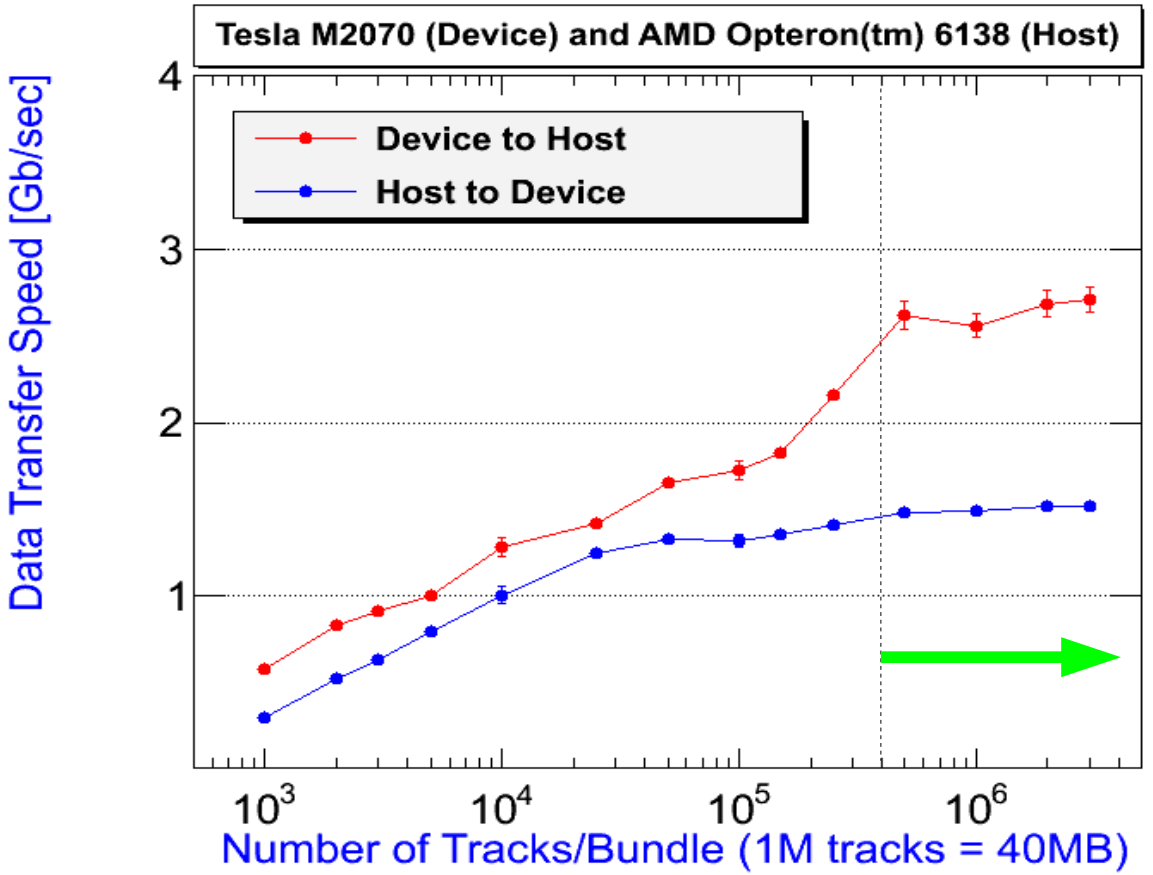

cmsExp
Track data (step size, x, p)
DEVICE
HOST
Transportation
TransportationManager
PropagatorInField
Do-Loop : stepLength
GeometryManager
FieldManager
Navigator
ChordFinder
MagneticField
Fieldmap
Do-Loop : missDistance
MagIntegratorDriver
EquationOfMotion
Do-Loop : truncationError
MagErrorStepper
ClassicalRK4
N X 3 calls

Performance Measure

- Performance measurements in execution time
  - 1 CPU vs. 448 GPU cores
  - cuda event timer (cudaEventElapsedTime)
  - GPU time = kernel execution + data transfer
  - default kernel: blocks=32, threads=128
  - default step size = 1cm
  - default size of tracks/bundle = 100K tracks
  - errors: RMS of measurements with 100 events

Performance: Data Transfer Rate

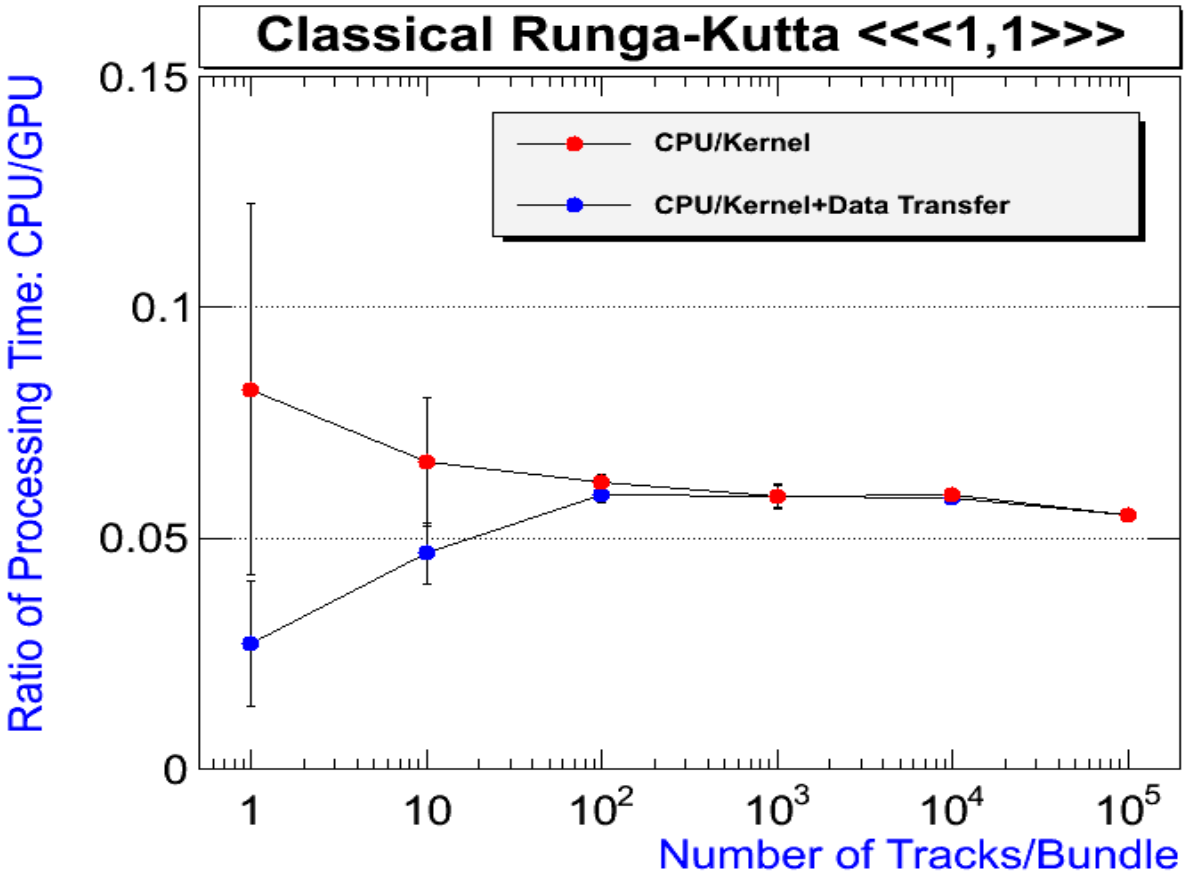
- Data transfer speed for track bundles between host and device



- Minimize data transfer between host and device
  - bandwidth device-device is $O(10^2)$ (GB/sec)
  - one large transfer is better than many small transfers

Baseline Performance: Single Thread GPU

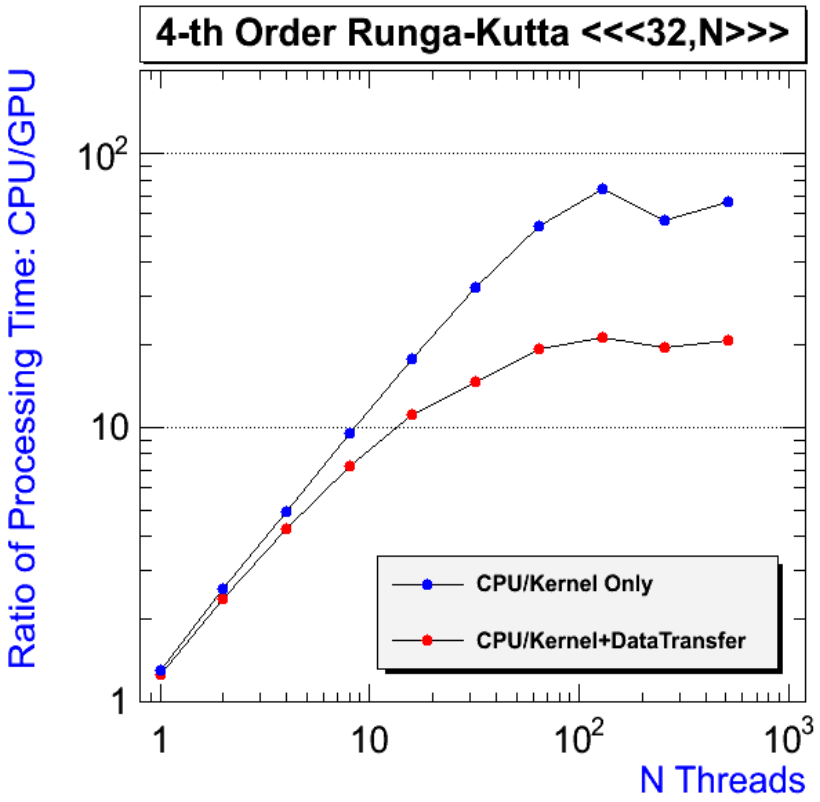
- <<<BLOCK=1,THREAD=1>>> for 4th order Runge-Kutta

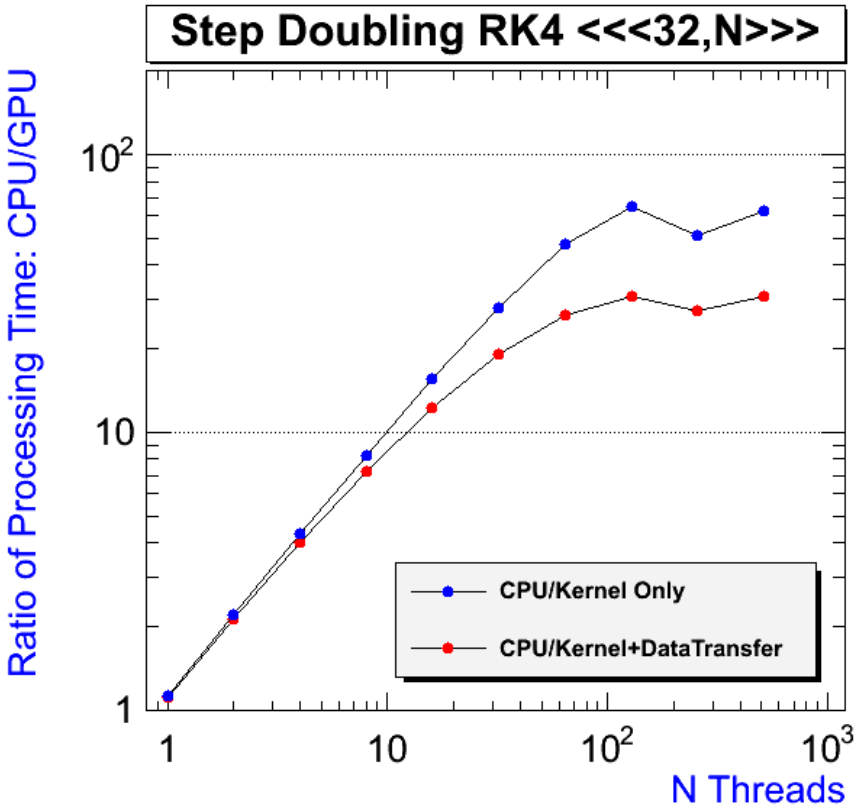


- Bottom line: 1 GPU core ≈ (1/18) CPU
  - clock speed (½), floating point calculation (¼), and etc.

Performance: Kernel with 32 Blocks

- RK4: Time(Kernel only) vs. Time(Kernel+data transfer)

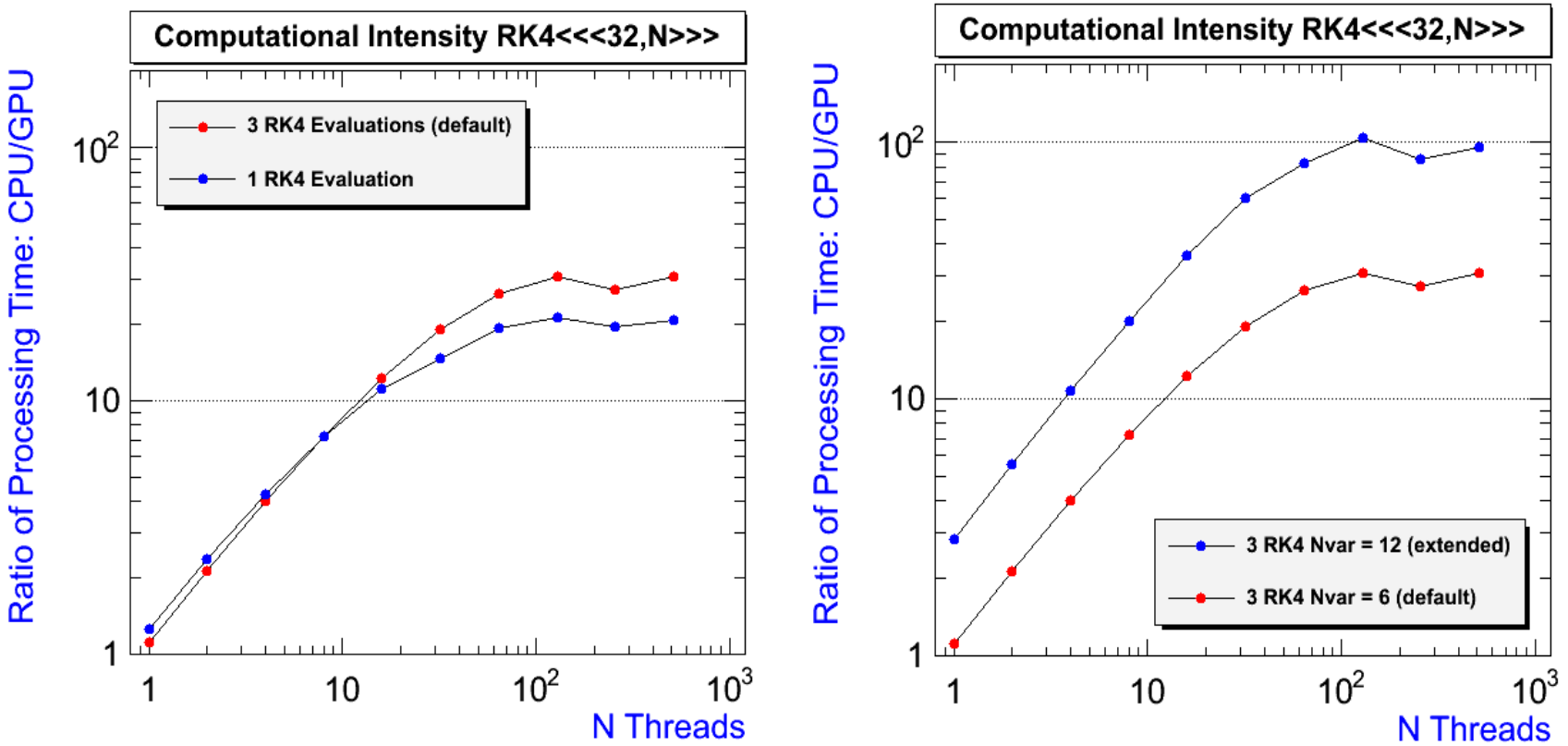




- Optimize kernel execution
  - overall (kernel+data)/kernel ~3 for RK4 and ~2 Adaptive RK4
  - minimize data transfer between host and device

Performance: Computational Intensity

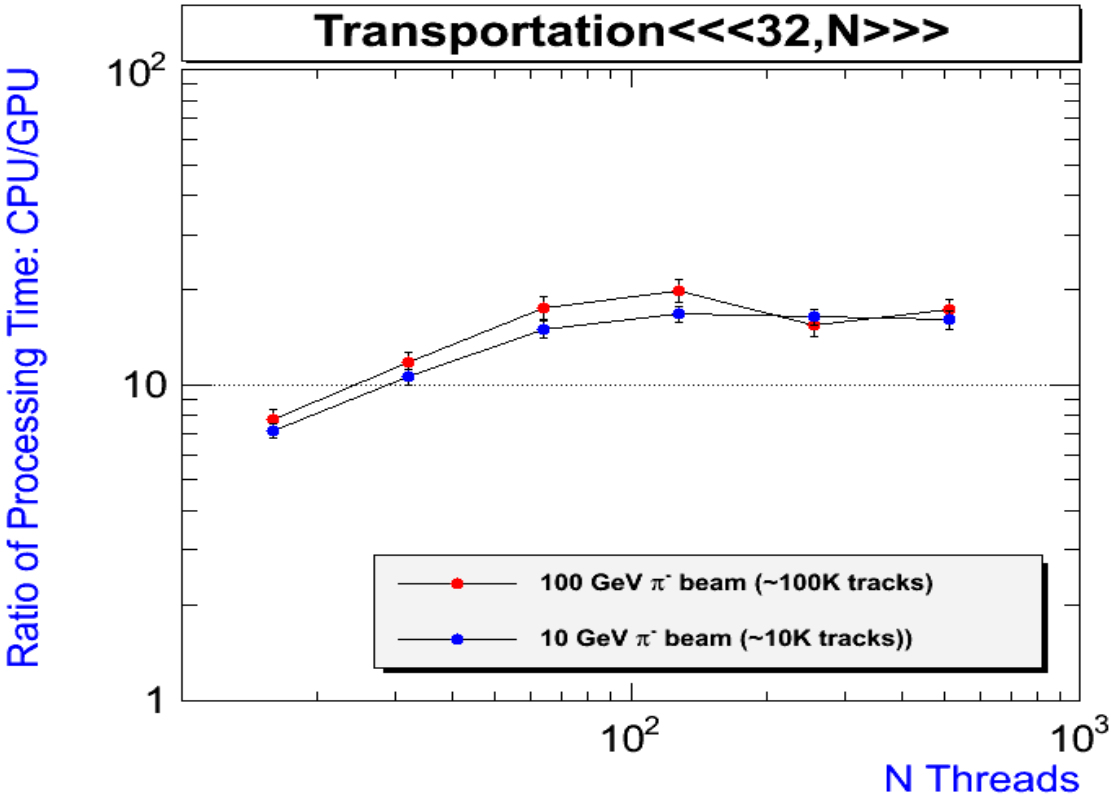
- Number of RK4 evaluations and number of variables



- Optimize arithmetic with computational intensity
  - do more arithmetic calculations on GPU
  - maximize independent parallelism (more for-loops)

Performance: Realistic Data from cmsExp

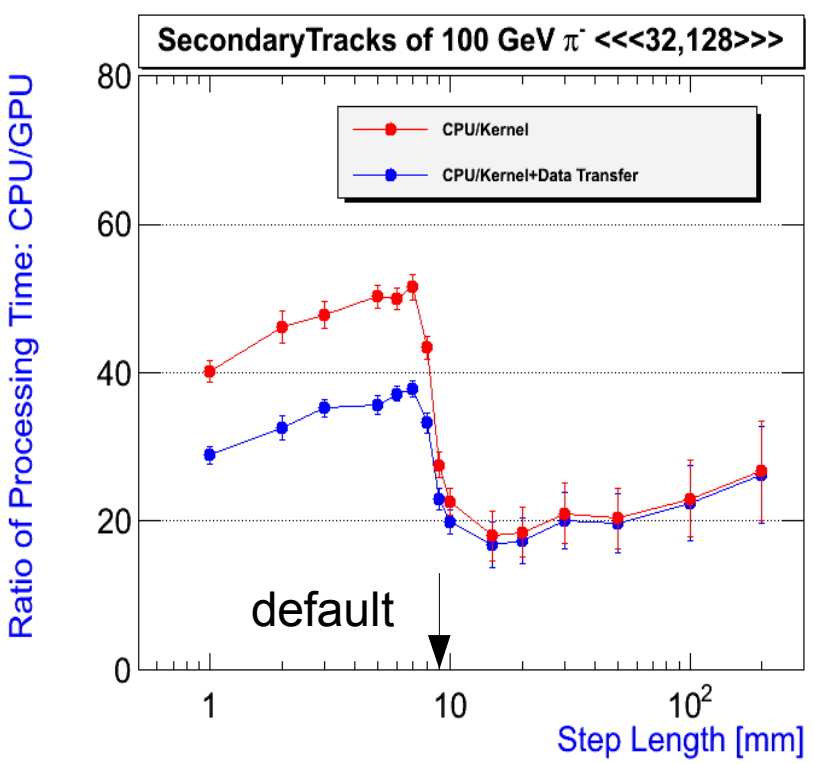
- CPU/GPU for the first step transportation for secondary particles produced by 10 GeV pions and 100 GeV pions
- Full chain of transportation with a step length = 1cm

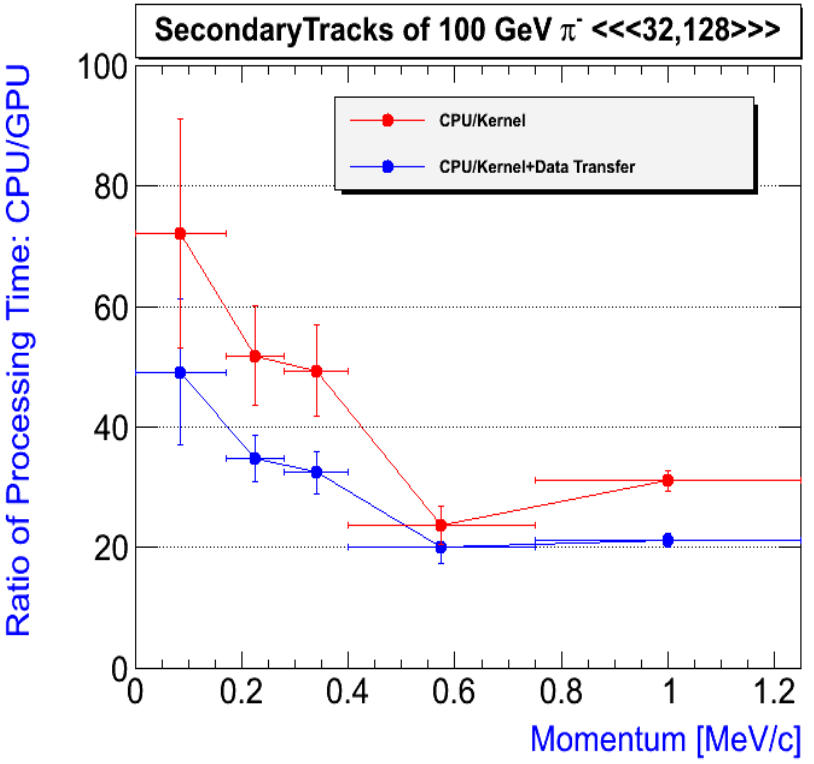


- Need additional arithmetic logistics to improve the gain

Dependence: Momentum and Step Length

- CPU/GPU for the first step of secondary tracks

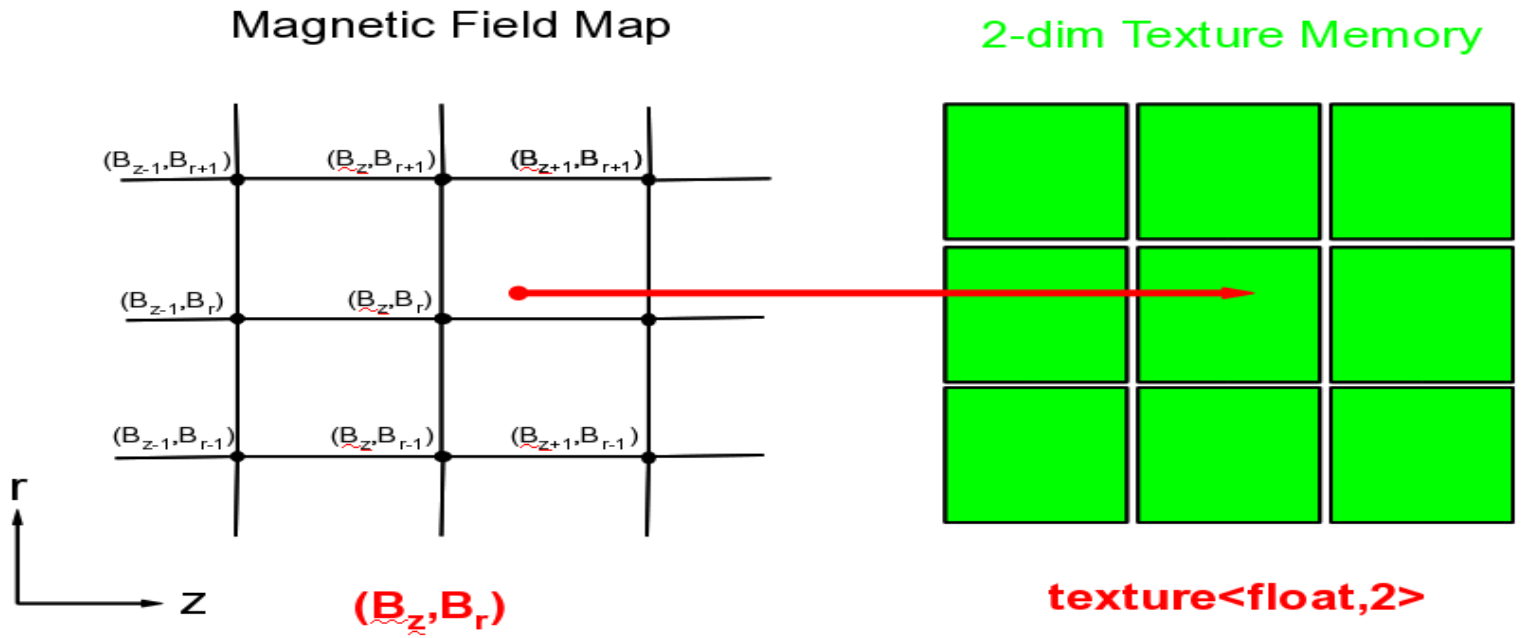




- Optimize calculation uniformity
  - Keep GPU multiprocessors equally busy
  - group tracks with same number of RK4 evaluations as possible

Magnetic Field Access : Texture memory

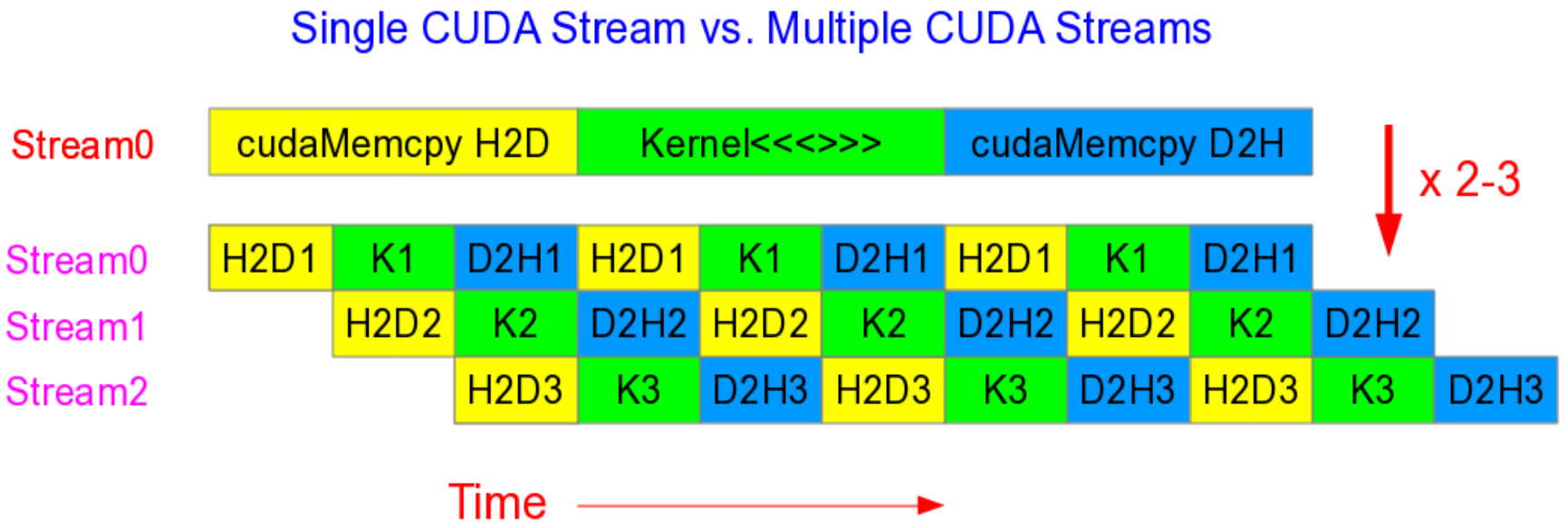
- Texture memory is cached on chip and designed for memory access with spatial locality
- Magnetic field map is a typically 2(3)-dimensional grid



- Texture interpolation twice as fast as the explicit interpolation for random access
- No noticeable difference in real data for 3 evaluations of RK4 w/wo using the texture - input data are ordered

Concurrent Kernel/Stream

- Multiple CUDA streams provide the task parallelism (kernel execution and memory copies simultaneously)



- Using multiple CUDA streams for Runga-Kutta diriver
  - no significant gain observed: balance work load evenly
  - Callgrind and IgProf profiling shows that there is only 40% more work to be gained without any geometry
  - add more calculations on device

Conclusion I

- A core part of Geant4 particle transportation has been tested on GPU
  - ratio of processing time for CPU/GPU ~ 20 with realistic data using 448 cuda cores
  - Identified key factors to maximize the GPU's ALU capacities
- Lessens learned
  - increase computational intensity on GPU
  - look for other transportation algorithms suitable for uniformity of calculations
  - organize input data for optimal efficiencies of kernel executions and data transfers

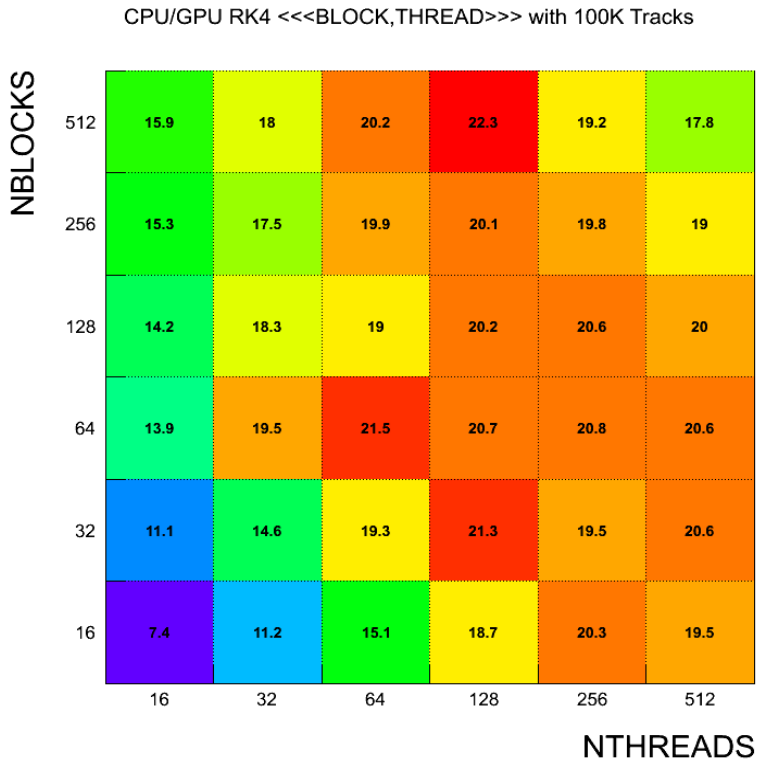
Conclusion II: Outlooks

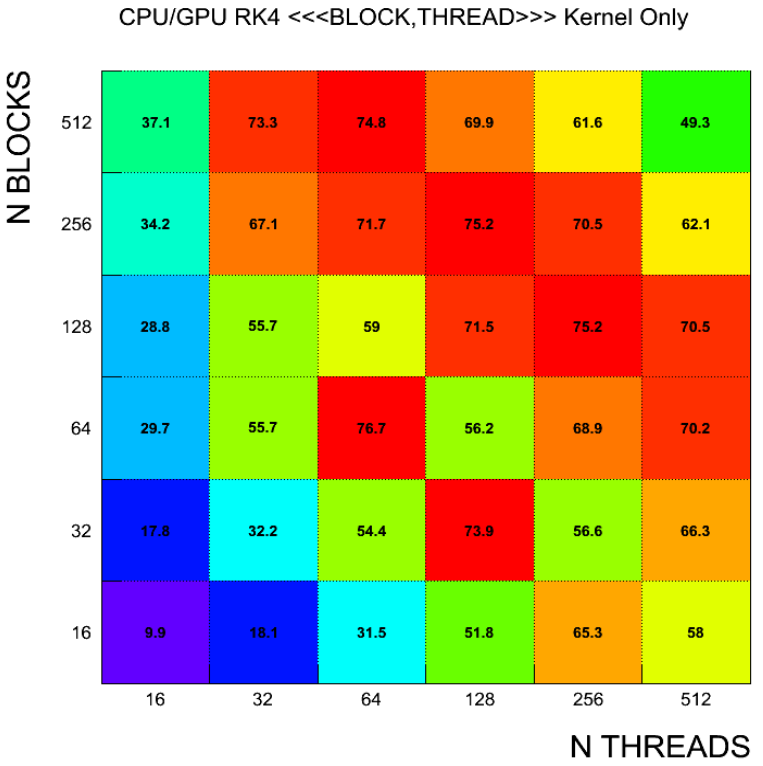
- Adding geometry on device
  - a simple detector (something like CMS crystals)
  - generalize transportation including photons and intersection with geometry
- Develop device codes for EM physics
  - multiple stepping on device to increase computations
  - generalize transportation including post step actions and pipelines for handling hits and secondaries
- Optimize GPU resources
  - more tests for multiple CUDA streams (concurrent kernel execution and copying data up/down to GPU)

Back-up Slides

Performance: CPU/GPU

- RK4: Kernel+Data Transfer vs. Kernel Only

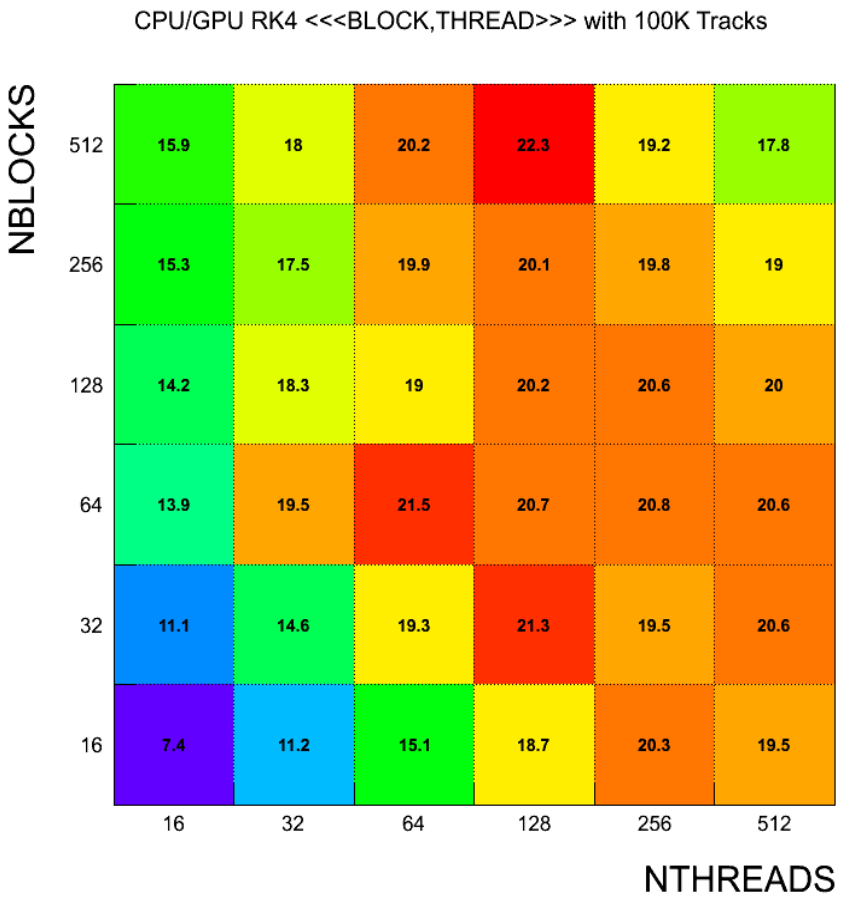


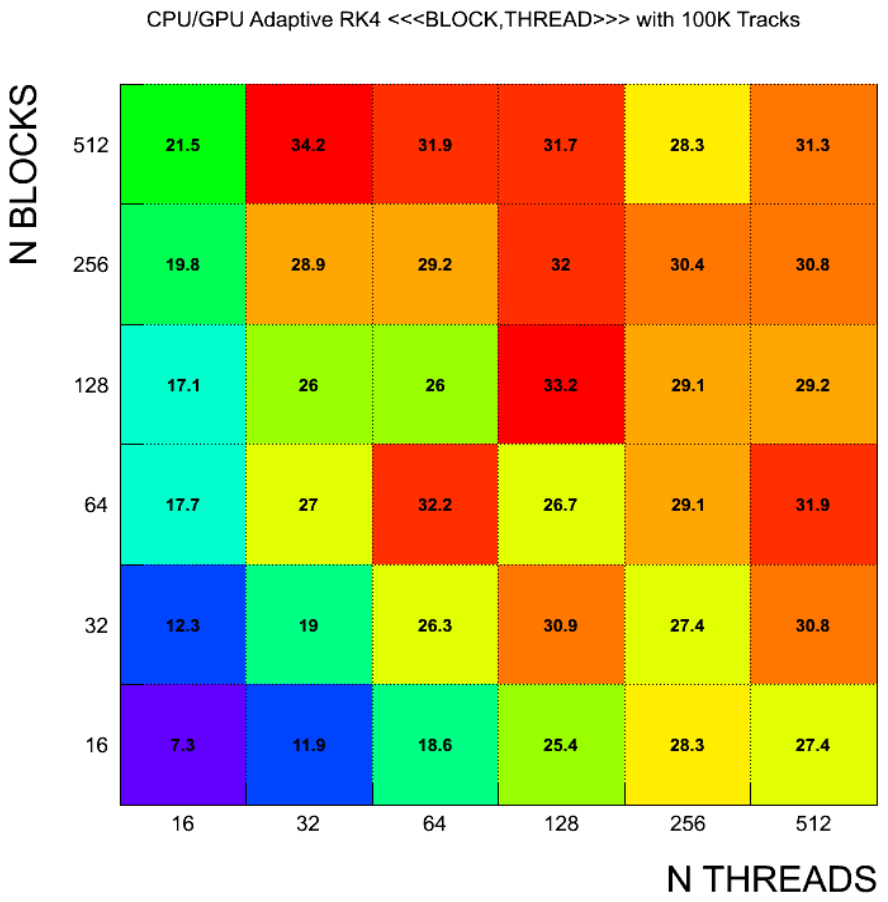


- Optimize Kernel Execution
  - Overall (Kernel+data)/Kernel = 3 for RK4
  - Minimize data transfer between host and device

Performance: Computational Density

- Number of RK evaluations: 1-RK4 vs. 3-RK4

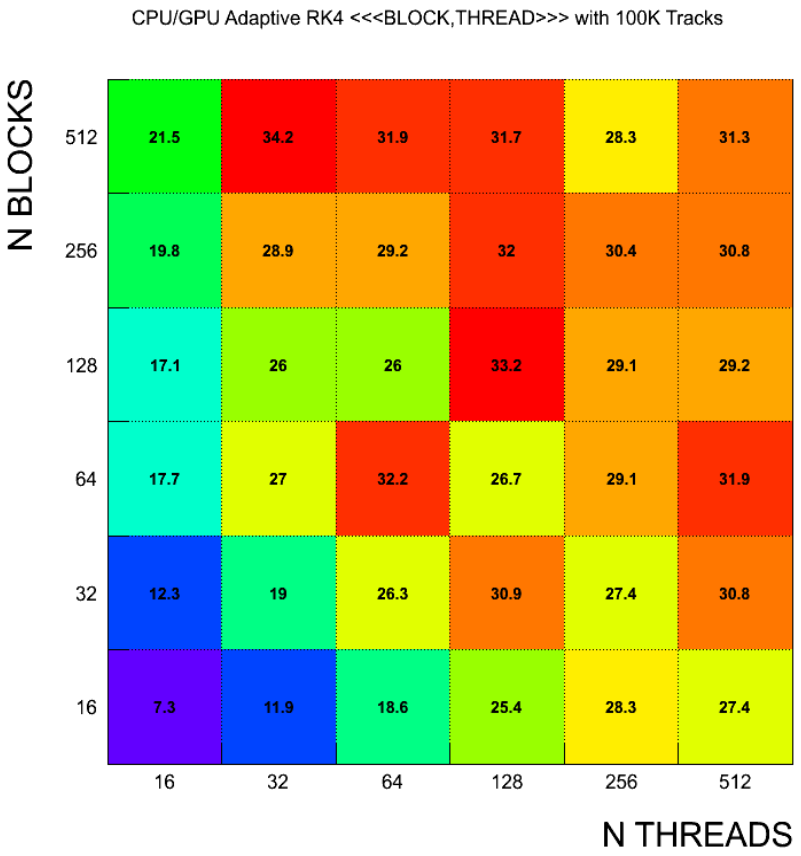


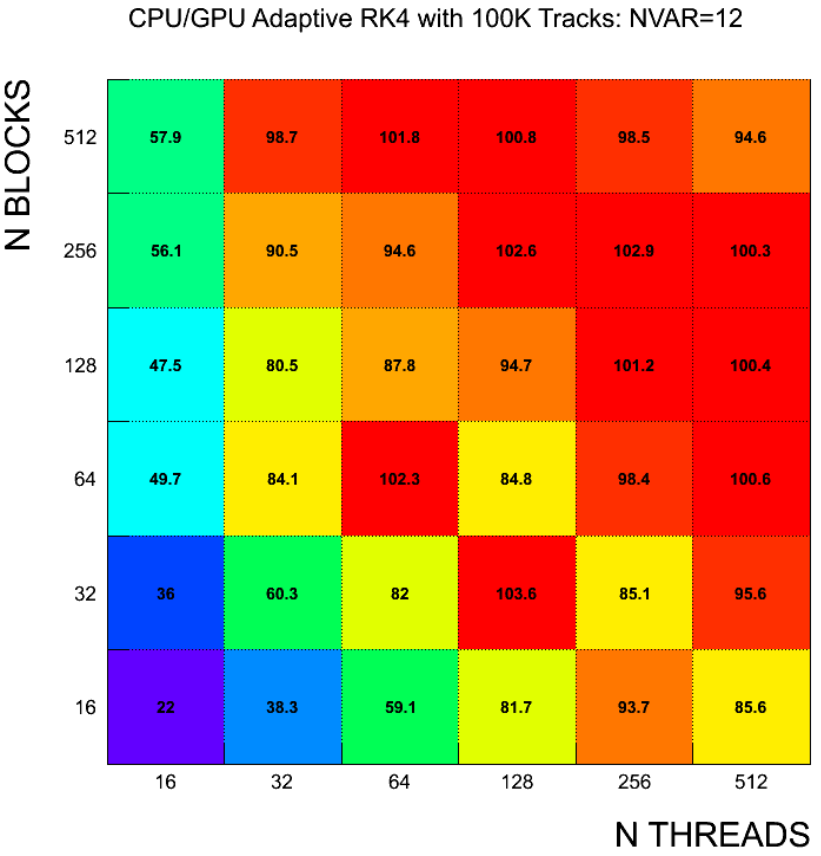


(Left) one RK4 evaluation (Right) three-RK4 evaluations

Performance: Computational

- Number of variables in equation of motion: 6 variables (default) vs. 12 (extended) for adaptive RK4.





- (Left) 6 variables (x,p) (Right) 12 variables (x,p,t,s)

Performance: Simulation Data with cmsExp

- CPU/GPU for the first step transportation for secondary particles produced by 10 GeV pions and 100 GeV pions
- Full chain of transportation with a step length = 1cm