Electromagnetic Physics Models for Parallel Computing Architectures

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Introduction

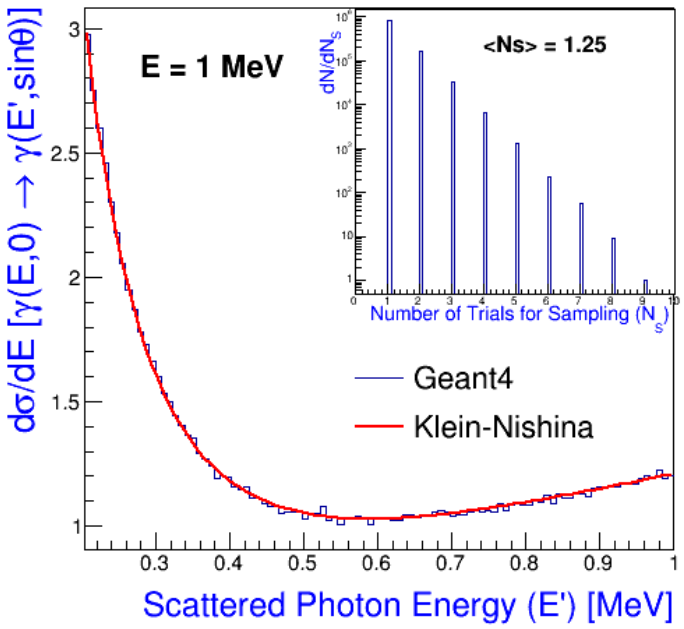
- Challenges and opportunities for HEP computing
  - ever-increasing computing power for future HEP programs
  - evolving hardware architectures and software technologies
  - promoting use of common resources and solutions to tackle next generation hardware (Forum for Computational Excellence) and advancing HEP community software (HEP Software Foundation)
- GeantV as next-generation detector simulation
  - simulation is one of the most CPU-intensive tasks in HEP computing and is largely experiment independent
  - concurrent framework for modern architectures, parallelized geometry and particle transport algorithms (track-level-parallelism)
  - see “GeantV: from CPU to accelerators”, by Andrei Gheata
- EM physics models for parallel computing architectures
  - 80% of CPU time is spent on electrons and photons in Geant4 for typical collider experiments, of which ~30% is on EM processes

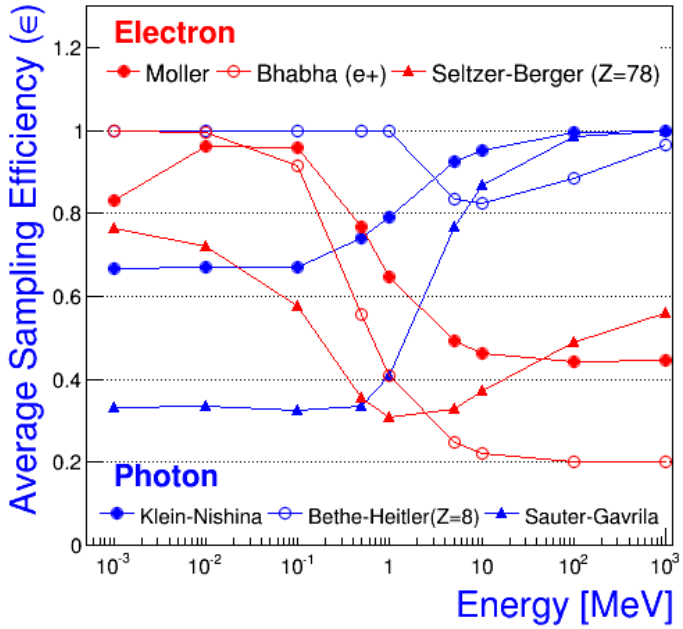
Challenges and Goals

- Characteristics of conventional HEP detector simulation
  - instructions are not reused often (many methods needed for each track, each with several branches)
  - memory bounded applications (cross section data, physics tables, geometry lookups, magnetic fields) – caching/locality
- No magical single solution for real world problems
  - particle transport in matter is an integral process (complexity)
  - explore every corner of technologies (diversity)
- Goal: write EM models, to deal with multiple tracks, to be accurate, fast and "portable"
  - maximum throughput for given resources
  - exploit both SIMD (vector pipeline) and SIMT (accelerators)
  - common source code between scalar, vector and accelerator (GPU, Xeon Phi)

Example of Algorithm Consideration: Sampling Methods

- Geant4 typically uses composition and rejection methods
  - accurate outcomes (ex. Compton at $E\gamma$ = 1MeV)
  - average sampling efficiency (ε) for photons and electrons

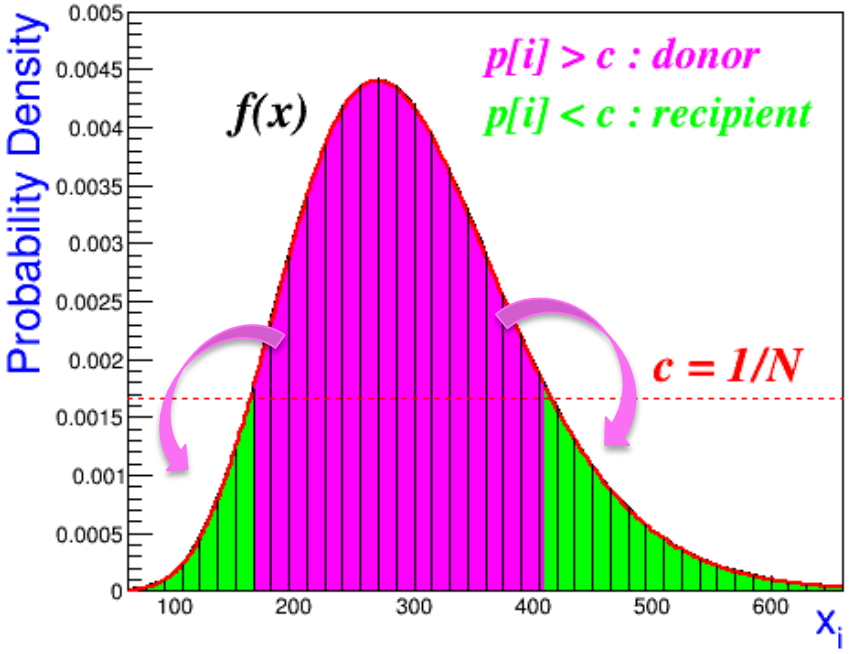


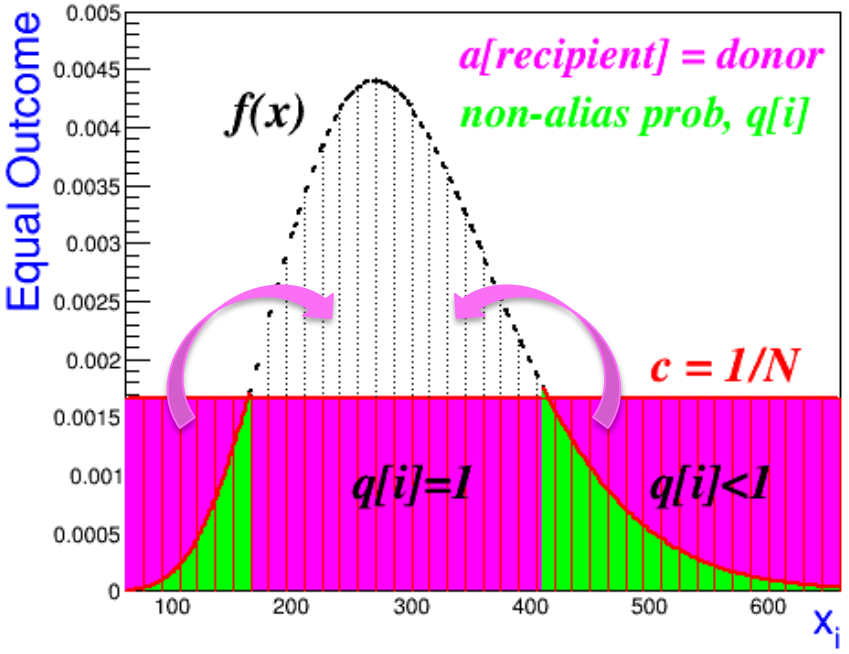


  - intrinsic problem for SIMD/SIMT: conditional branch (do-while)
  - probability to have the same number of trials for all n-vector operands (or n-threads) < $O(\varepsilon^n)$ (branch or thread divergence)
- Explore alternative methods to identify strengths (ability to vectorize), validity and limitations

Alias Sampling Method for N Discrete Outcomes

- Recast a N-discrete p.d.f to N equal probable events, each with likelihood 1/N = c (A. J. Walker, 1974) – effectively vectorizable
- Reproduce the original distribution by one trial sampling:
  - alias, a[recipient] = donor
  - non-alias probability, q[i] = probability not to take alias
  - for any random (xi), accept if rand(0,1) < q[i] or take the alias





Implementation Details

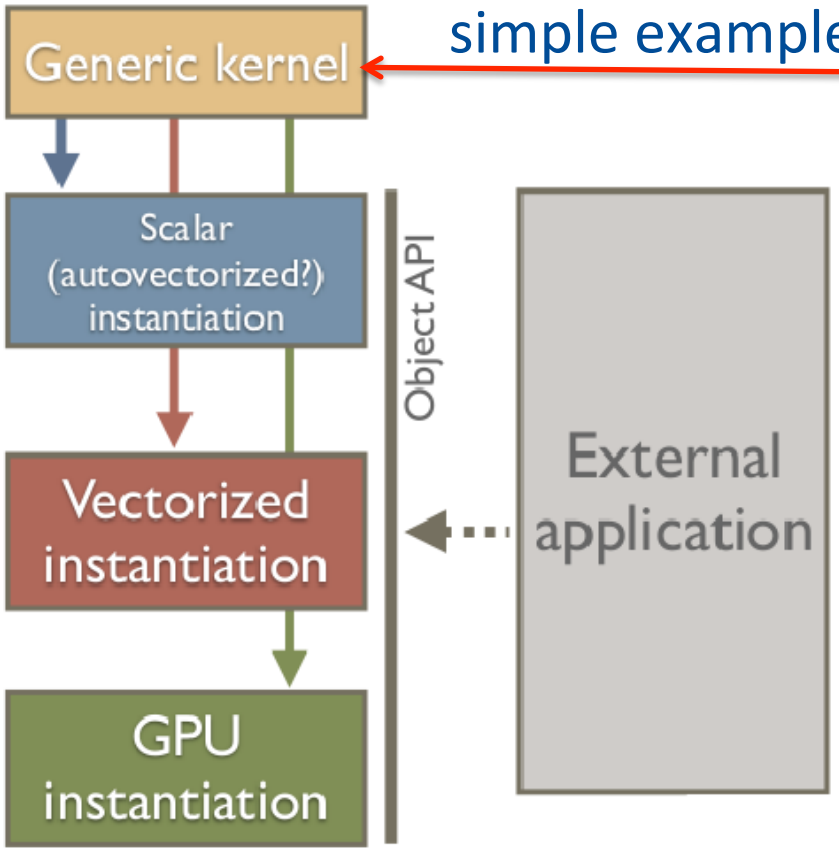
- Alias table: {a, q, p} [input-energy-bin][sampling-variable-bin]
  - equal log-division for input-energy bins
  - use cross section weighted bin positions (on the sampling axis)
  - for atomic dependent models, build tables for necessary elements
- EM physics models studied and size of sampling tables

Particle	Process	Model	Secondaries	Sampling Bin	Table Size
γ	Compton	Klein-Nishina	e^-	linear	100×200
	Conversion	Bethe-Heitler	e^-e^+	linear	$100\times100\times16$
	Photoelectric	Sauter-Gavrila	e^-	linear	100×200
e^-	Ionization	Moller-Bhabha	e^-	linear	100×100
	Bremsstrahlung	Seltzer-Berger	γ	log	$100\times100\times16$

- Sampling
  - table is chosen randomly from the ones below/above input-E
  - uniform sampling within a bin or a linear interpolation using p.d.f

Consideration for Portability: Scalar, Vector, CUDA

- Common interface to different architectures
  - generic kernel using abstract types (by backend)
  - template specialization
  - Technique pioneered in VecGeom (see also A. Gheata's talk)



simple example

```
inline namespace VECPHYS_IMPL_NAMESPACE { //cxx, cuda, ...

template<class Backend>
VECPHYS_CUDA_HEADER_BOTH
typename Backend::Double_t
GUAliasSampler::
SampleX(typename Backend::Double_t rangeSampled,
        typename Backend::Double_t probNA,
        typename Backend::Index_t  aliasInd,
        typename Backend::Index_t  icol,
        typename Backend::Double_t fraction) const
{
  typedef typename Backend::Bool_t   Bool_t;
  typedef typename Backend::Index_t  Index_t;
  typedef typename Backend::Double_t Double_t;

  Double_t r1 = UniformRandom<Backend>(ftate,fThreadId);

  Bool_t useDirect = (r1 <= probNA);
  Double_t binSampled = rangeSampled * fInverseBinSampled;

  Index_t      icolDist = icol;
  MaskedAssign(!useDirect, aliasInd, &icolDist); //if-else

  Double_t xd = icolDist*binSampled;
  Double_t xu = xd + binSampled;

  Double_t x = (1 - fraction) * xd + fraction* xu;

  return x;
}

} // end namespace impl
```

Other Considerations

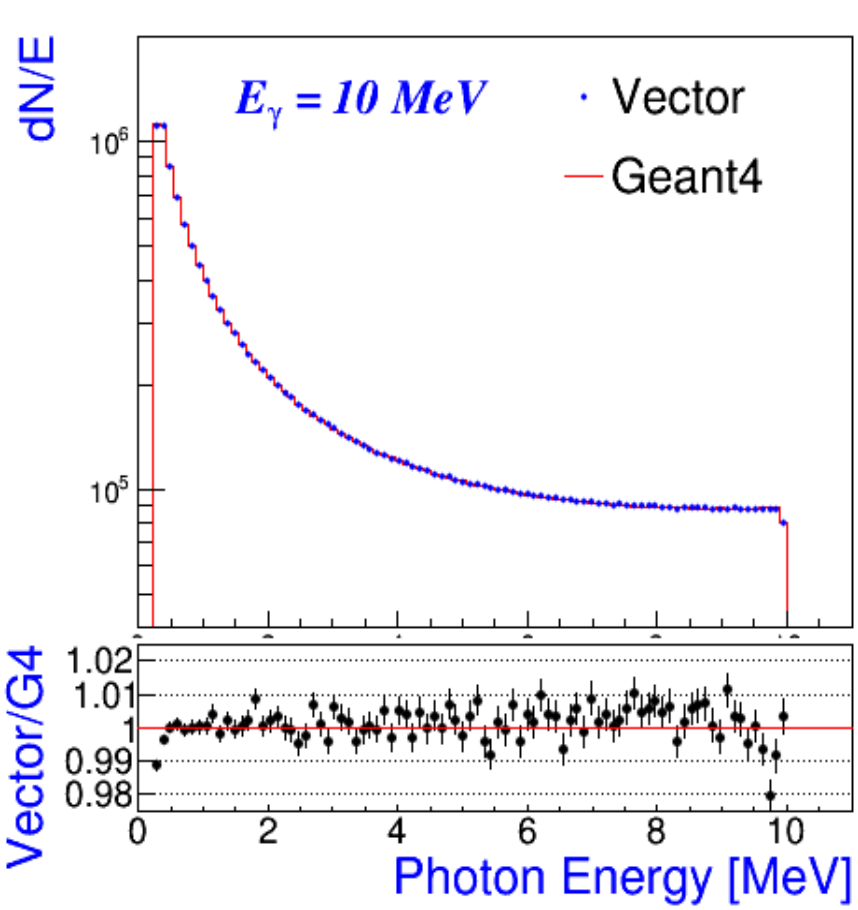
- Static polymorphism using CRTP (curiously recurring template pattern)
  - virtual is not allowed for template<backend>
  - avoid virtual layers (use early binding)
- Core techniques and patterns for vectorization: Vc library
  - conditional branches: mask
  - use gather to fetch data and place it contiguously
- Data structure
  - SoA (for vector) and AoS (for scalar, cuda)
  - Pre-sorting tracks by energy to apply different algorithms across different energy regions (also may reduce latencies) - optional
- Random number generation
  - Vc random numbers
  - Cuda pRNG library (CURAND)

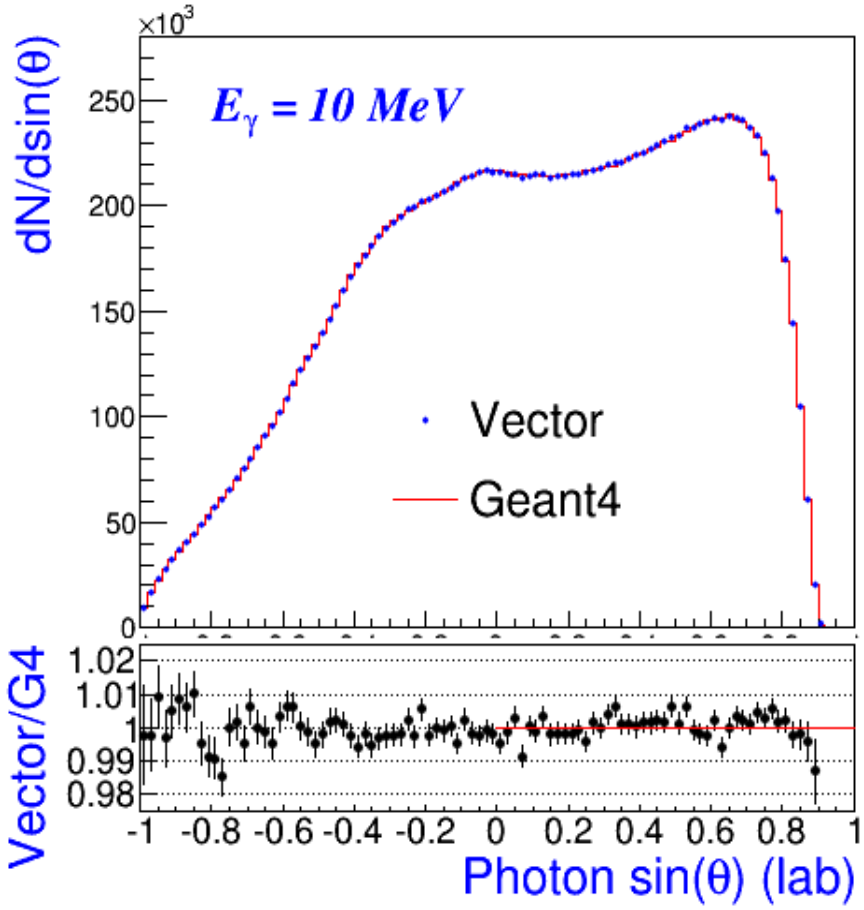
Preliminary Validation and Performance Evaluation

- Physics validation
  - simulate interactions at fixed input energy points
  - compare results (final states of interaction) w.r.t Geant4 (code extracted from Geant4)
- Performance measurement
  - 10 experiments, 100 repetitions per experiment
  - time for simulating N secondary interactions with a exponentially falling input energy spectrum in the range;
    - input energy range = [2MeV:20MeV] with 16 Z-elements
    - also tested in E [10keV:1MeV], E [10MeV:1GeV], E [10GeV:1TeV]
    - note that performance of Geant4 depends on the energy range
  - sample and store secondary particles, and update primary tracks
  - speedup = scalar/vector or scalar/GPU as the number of input particles (tracks) for the same task

Preliminary Validation: Alias Sampling Method vs. Geant4

- Compton: scattered photon energy and angular distributions with input photon energy = 10 MeV (Vector)

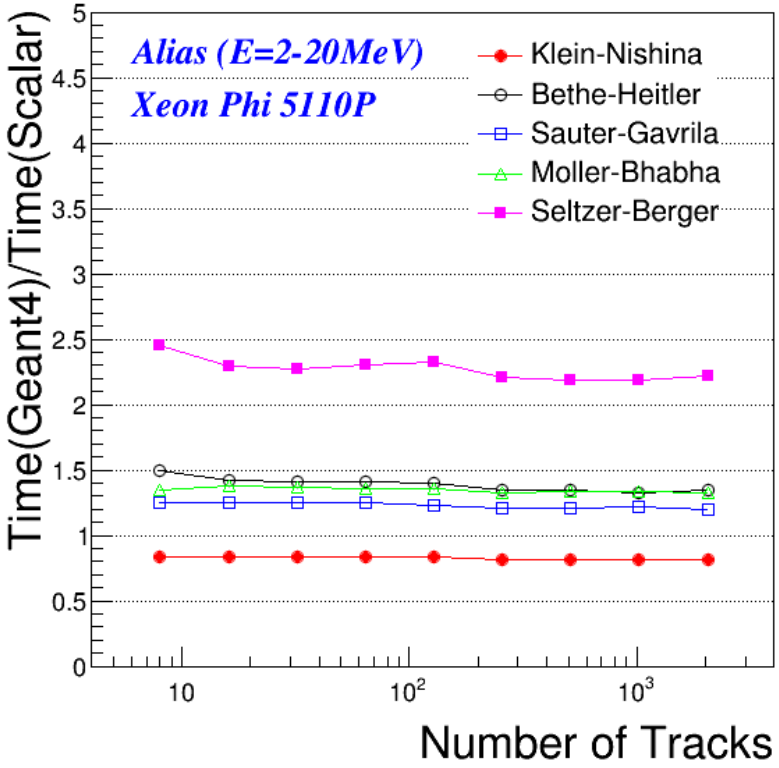


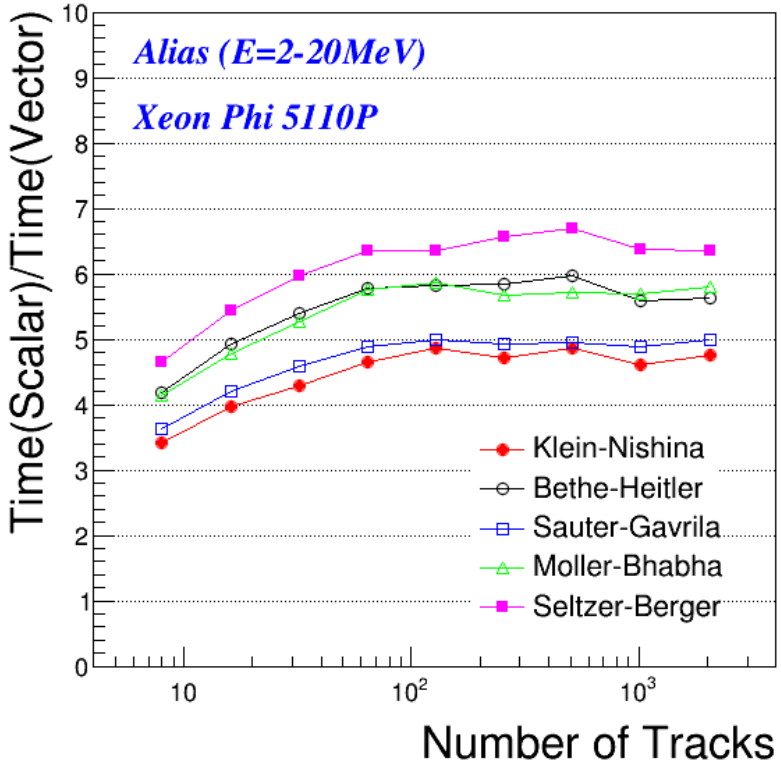


1%-level agreement up to 100 MeV with alias table size [100,200]

Preliminary Performance: Alias Sampling Method

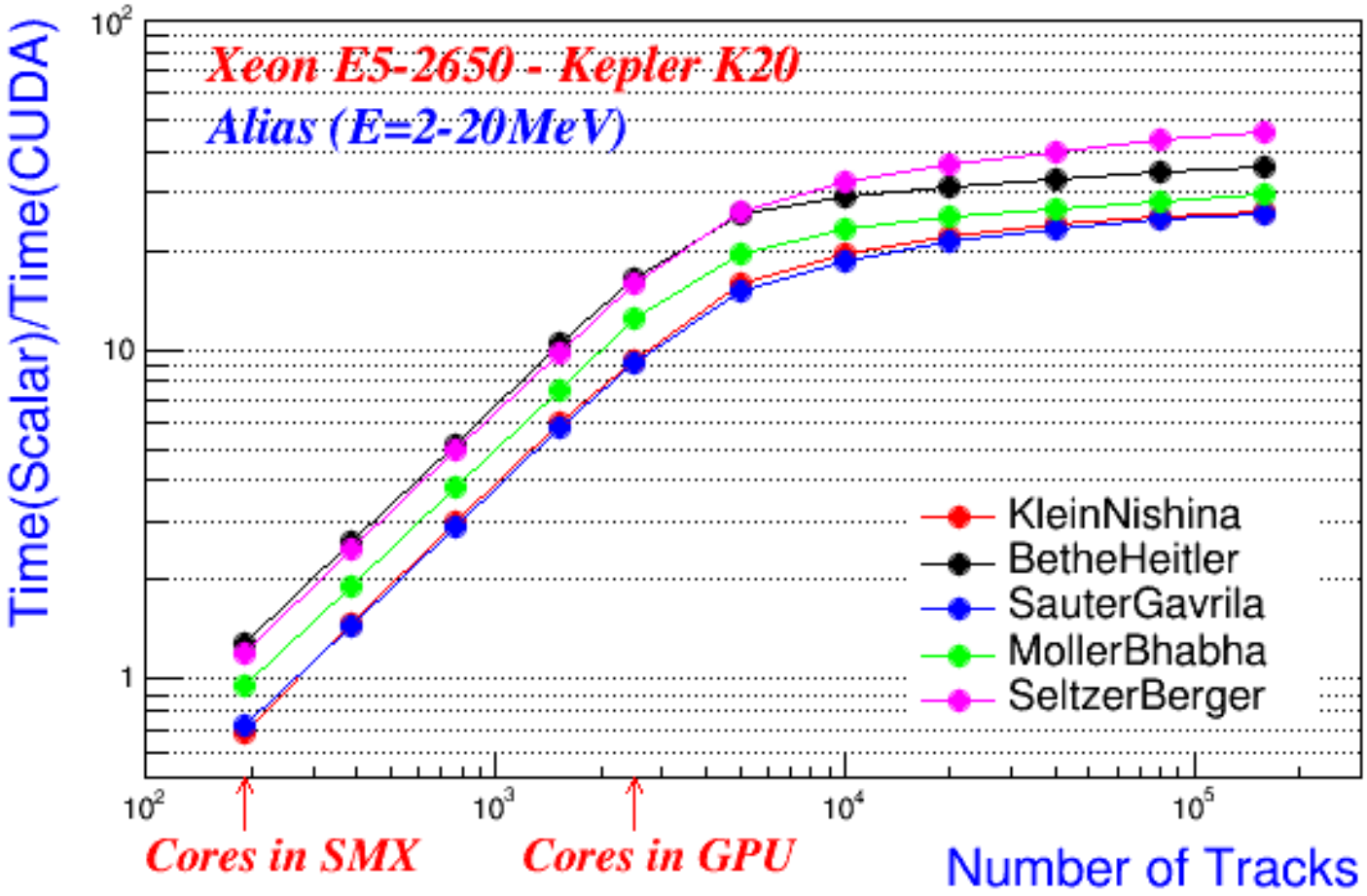
- Vector performance
  - input particle energy: 2-20 MeV (valid range for all models)
  - using 16 elements (random for each track)
  - MIC (Intel Xeon Phi 5110P 60 cores @ 1.053 GHz) - 8 vector pipelines for double precision – see also SSE/AVX in backup





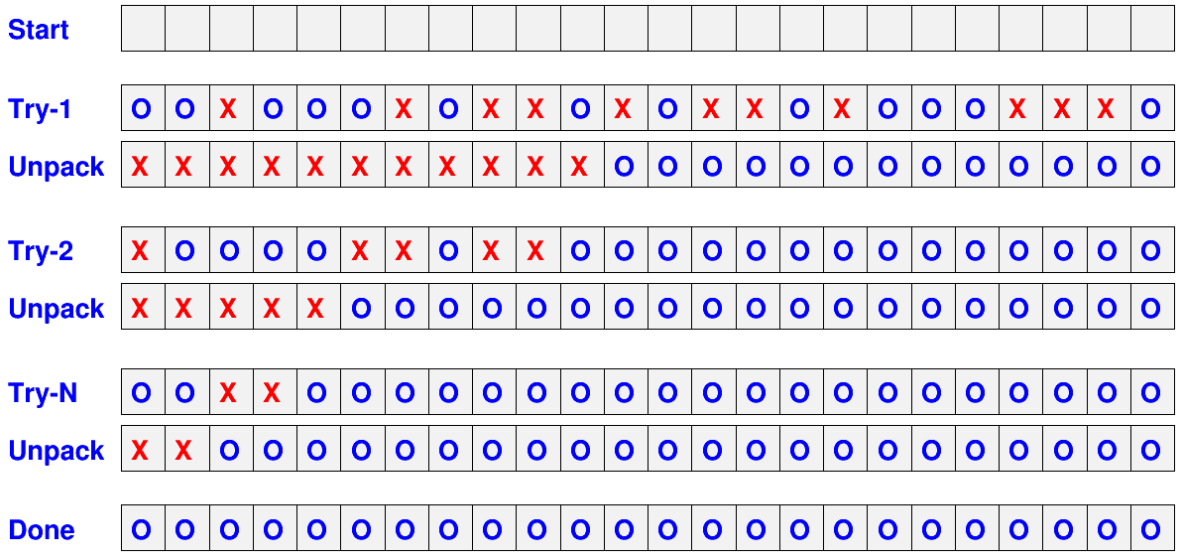
Preliminary Performance: Alias Sampling Method – GPU

- GPU
  - GPU: Nvidia Kepler (K20), 2496 cores @ 0.7 GHz - <<<26,192>>>
  - Host: Intel Xeon E5 – 2650 @ 2.60 GHz



Alternative Sampling Methods

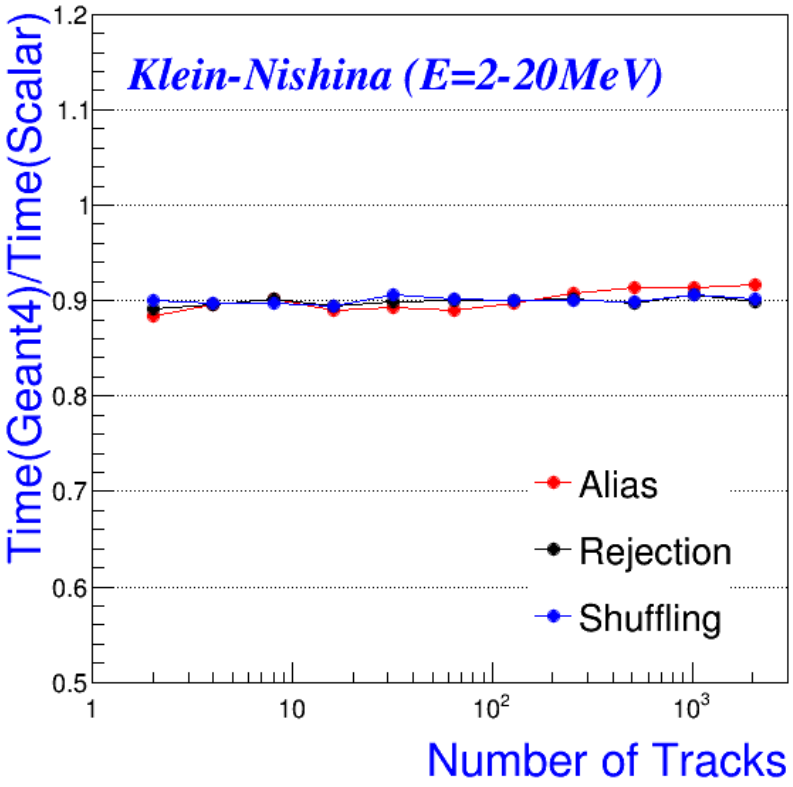
- Limitation of the discrete alias sampling method
  - the alias method with a finite bin size is subject to have biased outcomes if p.d.f is neither near constant nor linear within a bin
  - Ex.: $d\sigma/d\epsilon[\gamma(E,0) \rightarrow \gamma'(E', \sin\theta)] \rightarrow \epsilon^{-1} = E/E'$ for small ε
- Alternative techniques using the composition and rejection
  - Parallel (vector) + Sequential (scalar) loop - (see backup)
  - Shuffling (repeat try and unpack, overhead for reorganizing data)

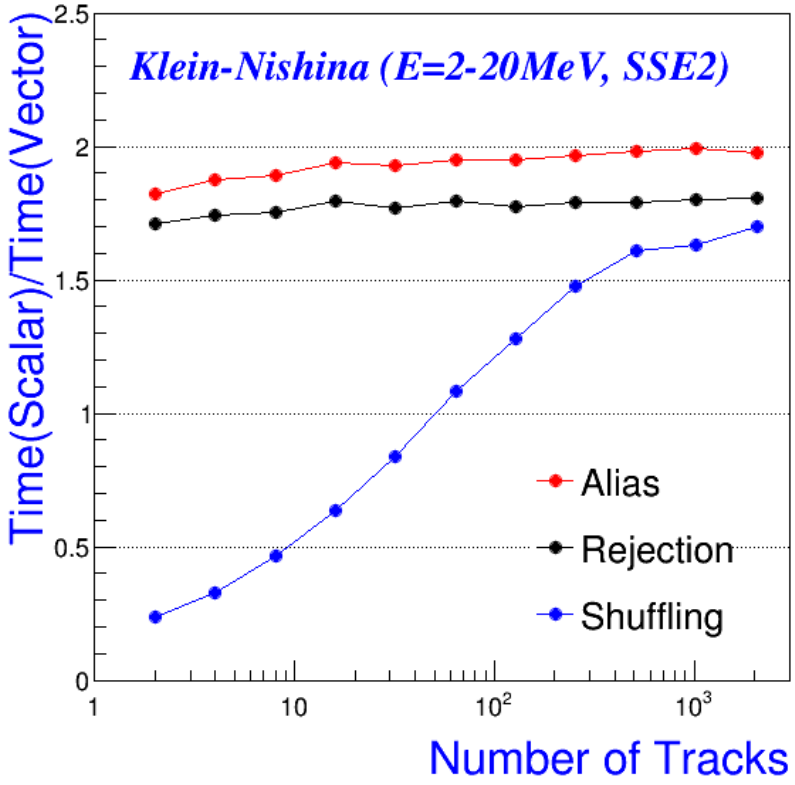


  - hybrid (mixture of different methods in the parameter space)

Performance: Alternative Sampling Method – Vector (SSE)

- Scalar/Vector
  - SSE (Intel Xeon E5 – 2650 @ 2.60 GHz) – SSE2





- Hybrid Compton for a small bucket of tracks
  - Alias [10keV,100MeV] + Rejection [100MeV,1TeV]

Summary

- Demonstrated feasibility of implementing electromagnetic physics models for SIMD/SIMT architectures with common source code
- Integrated different methods (alias, adaptions of accept/reject)
- Validating physics results with Geant4 and evaluating computing performance
- Outlook
  - optimize further for both SIMD and SIMT
  - Integrate in the GeantV framework
  - measure performance in full simulation

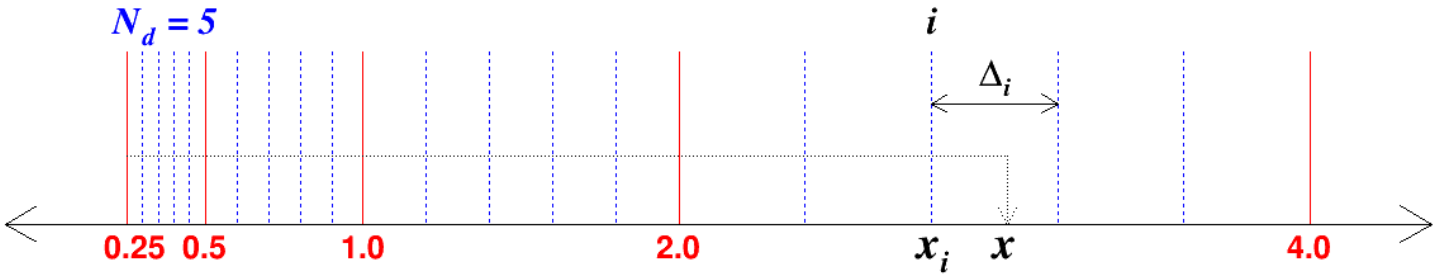
Backup Slides

Example of Performance Consideration: Binning Technique

- Construct bins (x_i) with a equal divisor (N_d) between the power of 2 from 2^{Nmin} to 2^{Nmax} for any integer N_{min} and N_{max}

$$x_i = [1. + (\frac{i\%N_d}{N_d})] \cdot 2^{\frac{i}{N_d}+\mathrm{N_{min}}}, \qquad i \in [0, (N_{max} - N_{min}) \cdot N_d + 1]$$

- For any x in [2^{Nmin}, 2^{Nmax}], the bin number (i) and the fraction (δ)



$$\begin{aligned} M &= \mathrm{frexp}(x, \&E) \\ i &= N_d \cdot (E - 1 - N_{min}) + \mathrm{floor}[(2M - 1) \times N_d] \\ \Delta_i &= [\mathrm{ldexp}(1., E - 1)]/N_d \\ \delta &= \frac{(x - x_i)}{\Delta_i}, \qquad \delta \in [0, 1) \end{aligned}$$

Random Number Generators

- Pseudo random number generator (pRNG)
  - Sequential: std::rand()
  - Vector: Vc Random_t
  - Cuda pRNG library (CURAND)
- Performance: 10K pRNG generation time in [ms]
  - CPU (Xeon x5650, 2.67GHz)

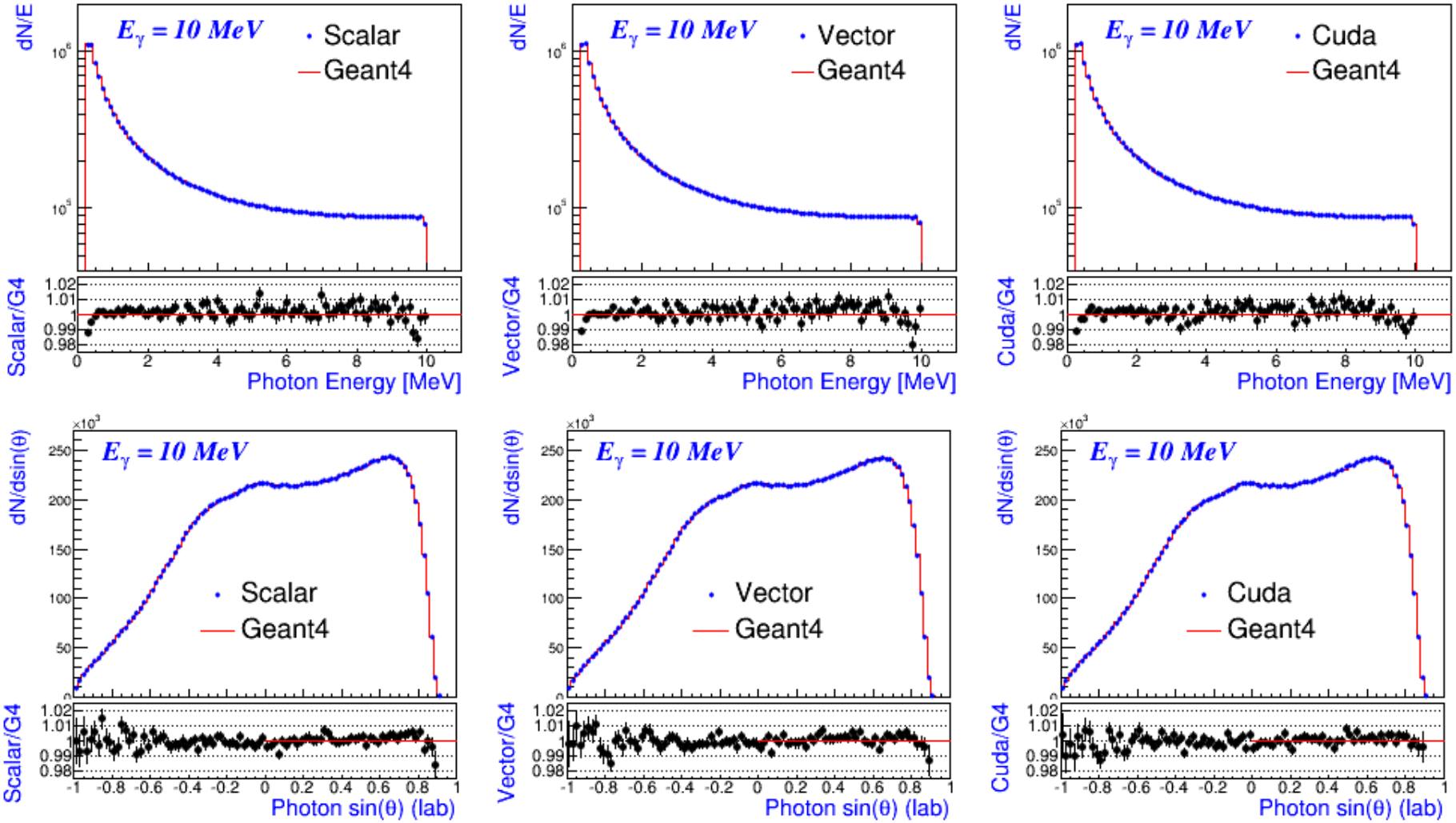
pRND generator	10K pRNG [ms]
Rand()	3.66
Vc random_t (SSE)	1.44

  - GPU (Nvidia K20M)

CURAND	Init States for 64 blocks [ms]	10K pRNG for 256 threads [ms]
XORWOW	4.12	7.92
MRG32k3a	5.02	21.88
MTG32	0.69	31.94

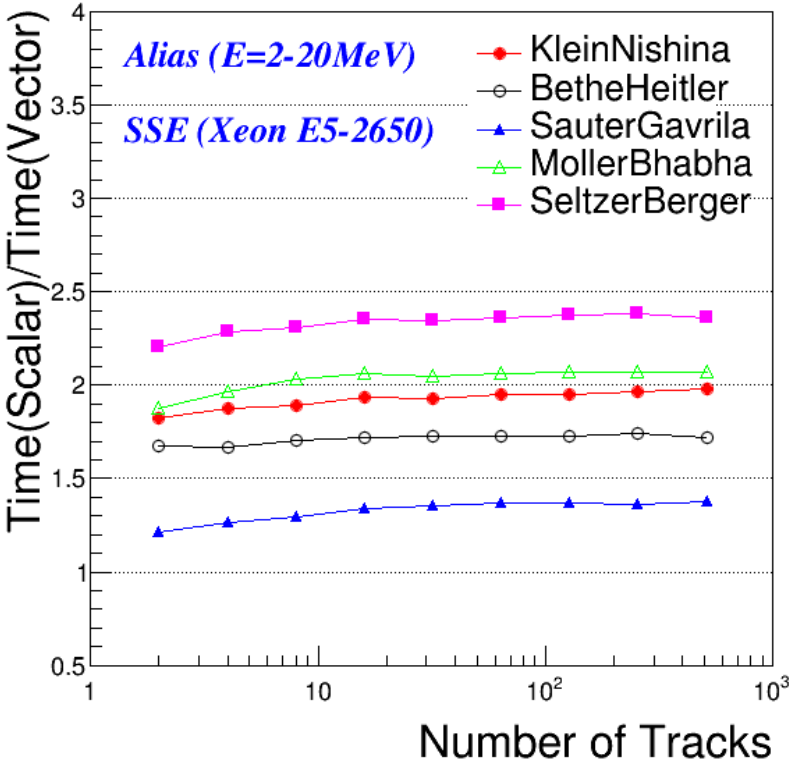
Preliminary Validation: Alias Sampling Method vs. Geant4

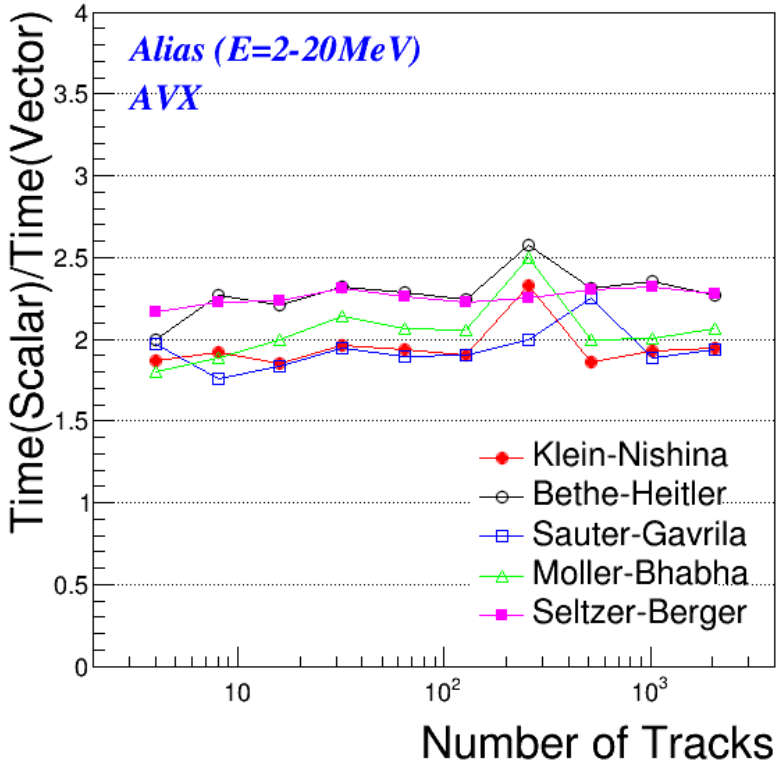
- Compton: scattered photon energy and angular distributions with input photon energy = 10 MeV (Scalar, Vector, Cuda)



Preliminary Performance: Alias Sampling Method – Vector

- Scalar/Vector
  - SSE (Intel Xeon E5 – 2650 @ 2.60 GHz) – SSE2
  - AVX (Intel Xeon E5 – 2620 @ 2.00 GHz)





Limitation of Discrete Alias Sampling

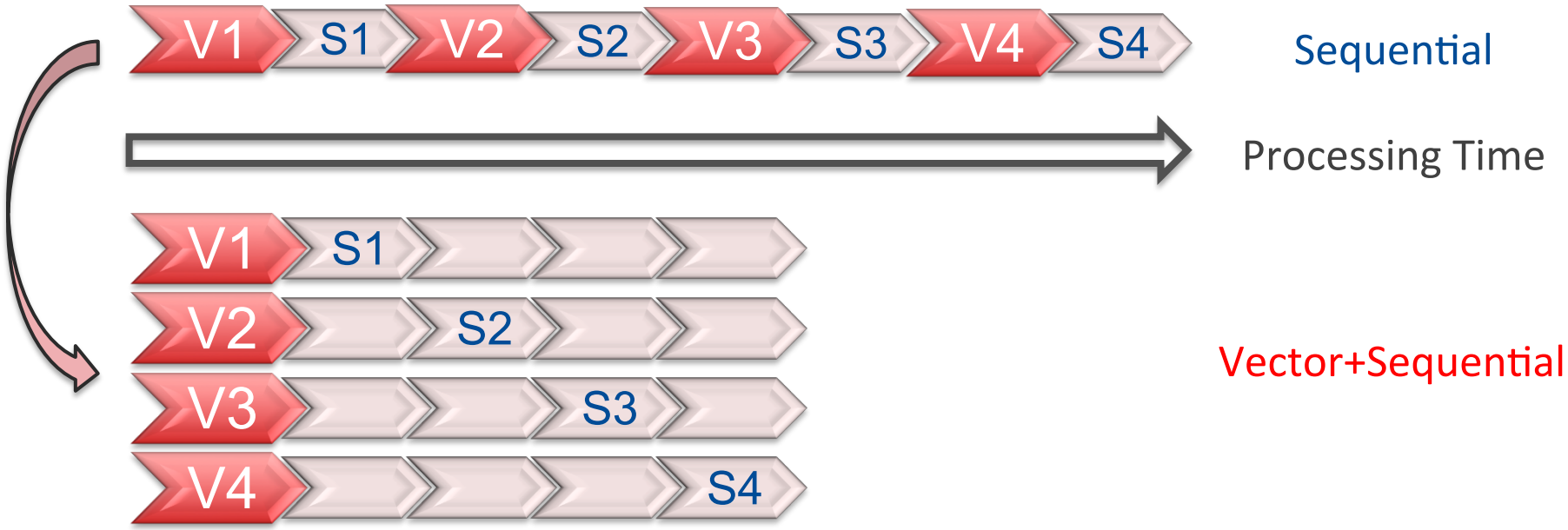
- The alias method with a finite bin size is subject to have biased outcomes if p.d.f. of sampling, f(x) is significantly non-linear within a bin
  - alias method may reproduce the average of f(x) within a bin (i.e, building alias tables at integrated averaged points and a interpolation within the sampling bin)
  - still no guarantee to sample g(f(x)) correctly even though <f(x)> is well reproduced
  - this is also true for the inverse cumulative approach
  - Example for Compton scattering: for large E and small E'

$$\frac{d\sigma}{d\epsilon}[\gamma(E,0) \rightarrow \gamma'(E', \sin\theta)] = \frac{X_o n \pi r_o^2 m_e}{E^2}[\frac{1}{\epsilon} + \epsilon][1 - \frac{\epsilon \sin^2\theta}{1+\epsilon^2}] \propto \frac{1}{E^2}\frac{1}{\epsilon}$$

$$\epsilon = \frac{E'}{E} = \frac{m_e}{m_e + E(1-\cos\theta)}$$

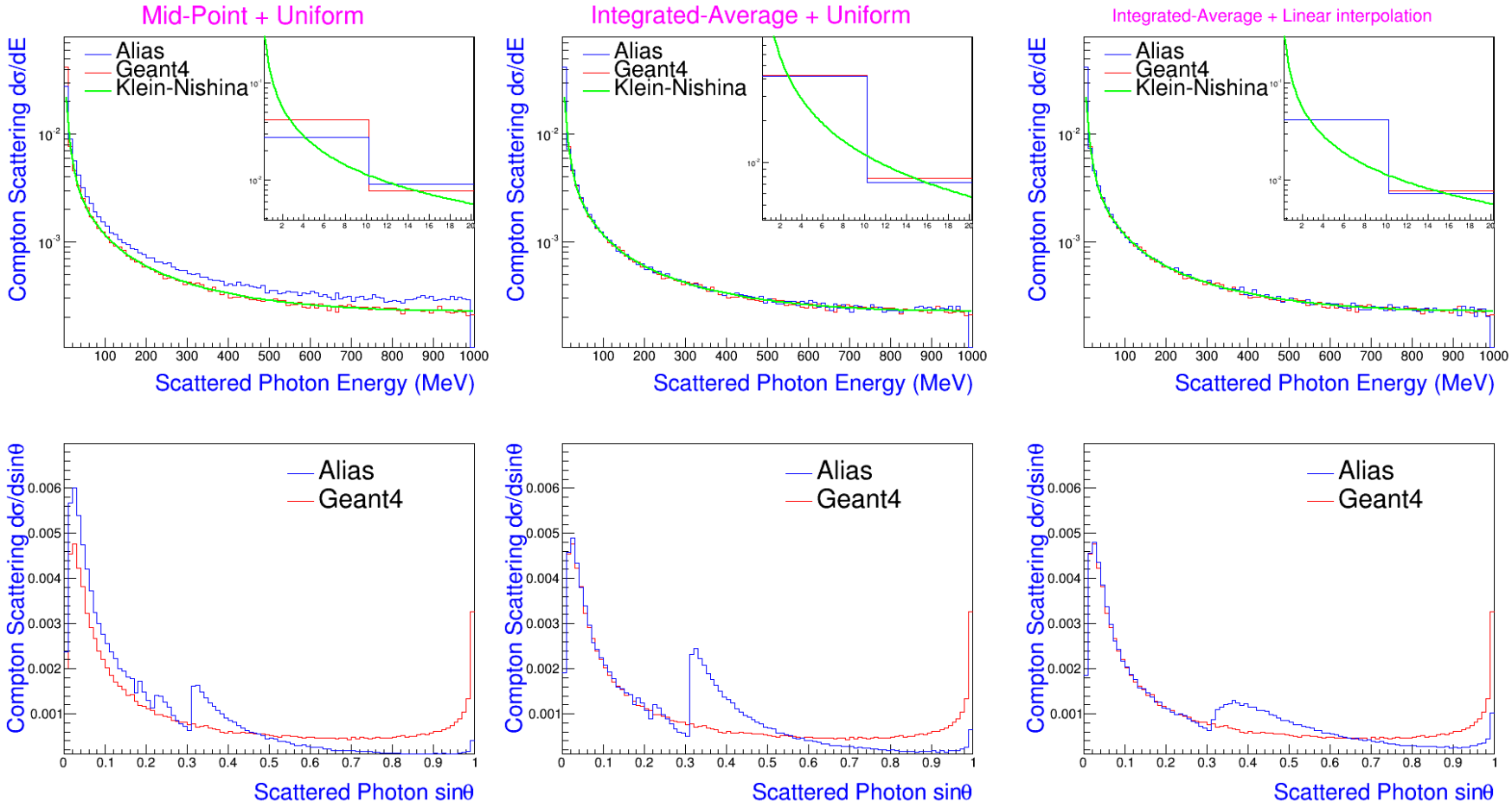
Vector + Sequential (Scalar) loop

- Sequential (scalar) operation for non-vectorizable (do-while) part of the composition and rejection method:
  - Amdahl's Speedup = 1/[(1-P) + P/N]
    where N = vector width for Vc and P = fraction of parallel code
  - Example with N = 4, V=vectorizable, S=sequential, P=V/(V+S)



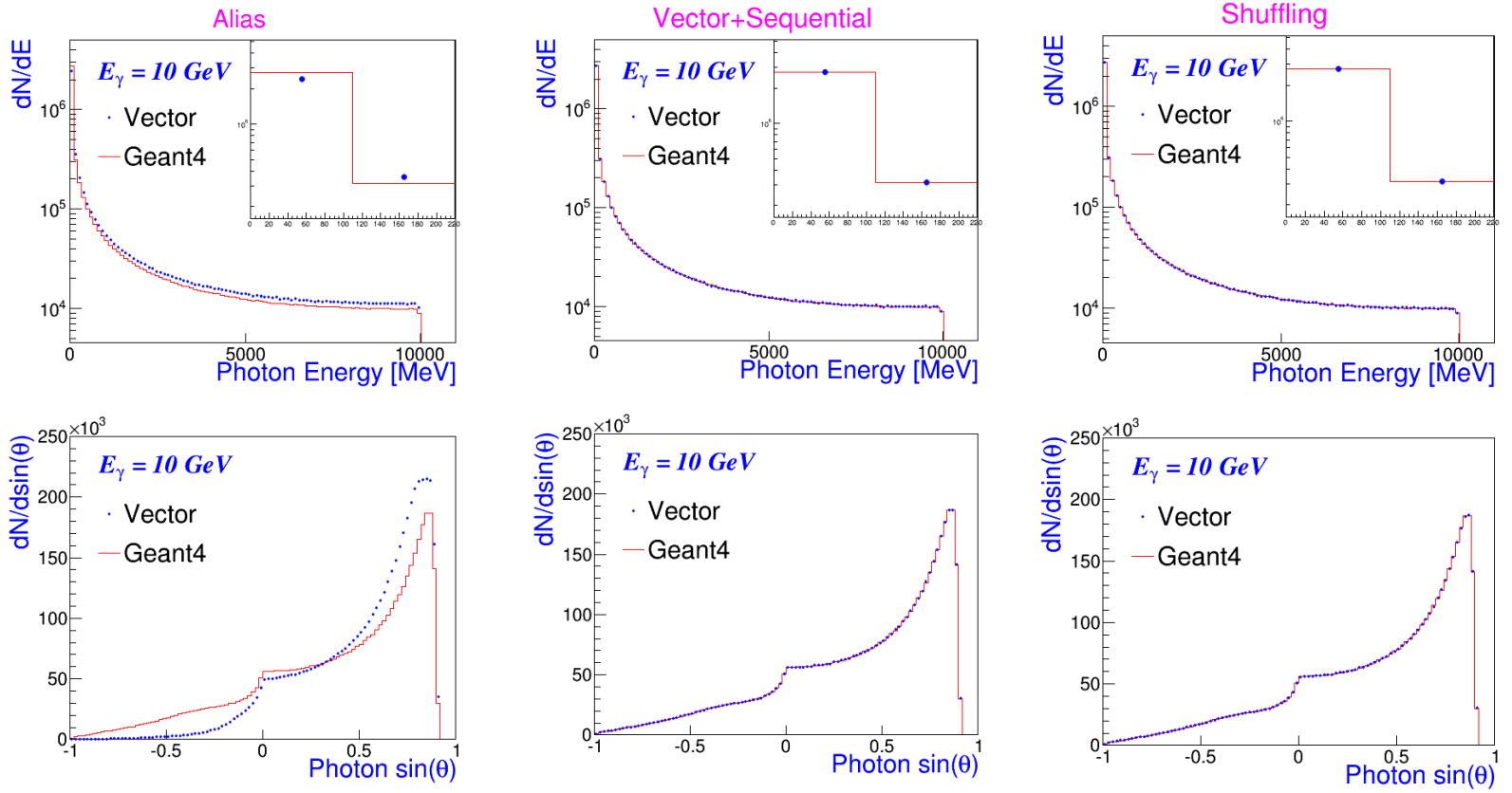
Limitation of Discrete Alias Sampling

- Compton scattering for Eγ = 1GeV
  - mid-point + uniform sampling
  - Integrated average + uniform sampling
  - Integrated average + linear sampling



Validation: Alternative Sampling Methods

- Compton scattering for input Eγ = 10 GeV: (Vector/Geant4)
  - Alias: Integrated average + linear sampling, table (100, 200)
  - Vector + Sequential
  - Shuffling method:



- Hybrid compton: alias (upto 100 MeV) + alternative method

Performance: Alternative Sampling Methods - GPU

- GPU
  - GPU: Nvidia Kepler (K20), 2496 cores @ 0.7 GHz - <<<26,192>>>
  - Host: Intel Xeon E5 – 2650 @ 2.60 GHz