

Accelerated Monte Carlo Particle Generators for the LHC

(MC@GPU)

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GPU DAY 2015
The Future Of Many-Core Computing in Science

OUTLINE

- MC generators in high-energy heavy-ion physics
- The biggest data challenge: LHC & WLCG with GPUs?
- GPU based PRNG for MC generators
- Performance tests by GPU based MC
- What can we learn from pp MC simulations?
- Outlook

MC generators in high-energy collisions

Why do we need Monte Carlo generators?

There are problems with no analytical expression, no closed form, or no deterministic description, like:

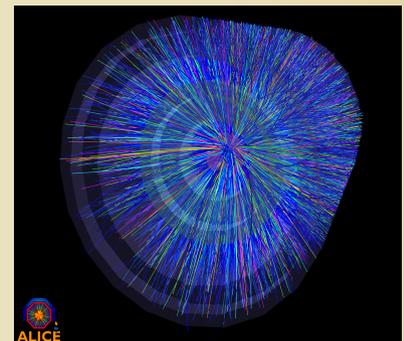
- stochastic processes (independent events)
- numerical (multi-D) integration
- optimization

Solution & errors

Random sampling of numerical results

Error estimation by standard deviation

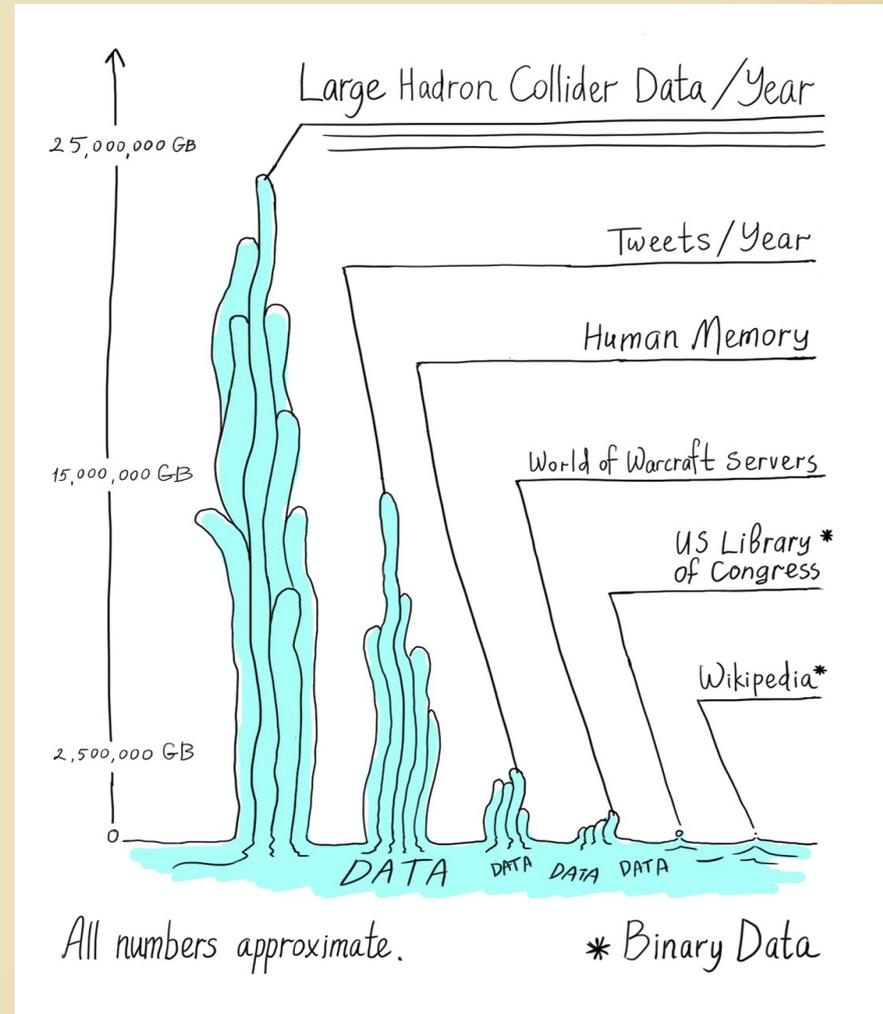
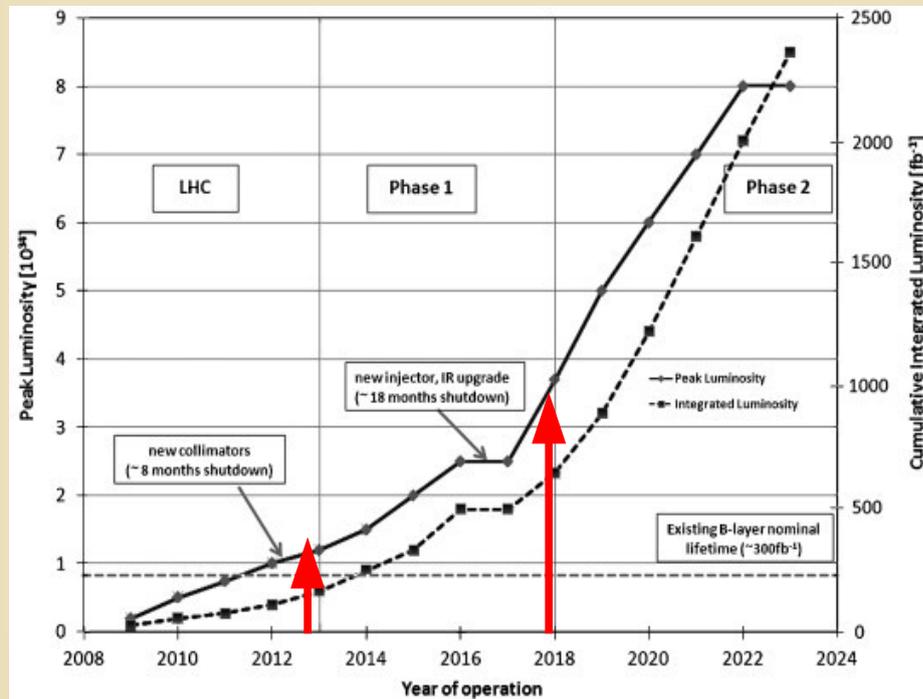
Fast random numbers → Computing & IT



The biggest data challenge: LHC

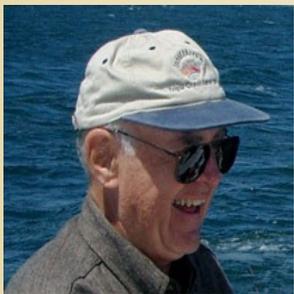
WLCG - Worldwide LHC Computing GRID:

15-20 Petabytes data per year
...and more after LHC upgrades

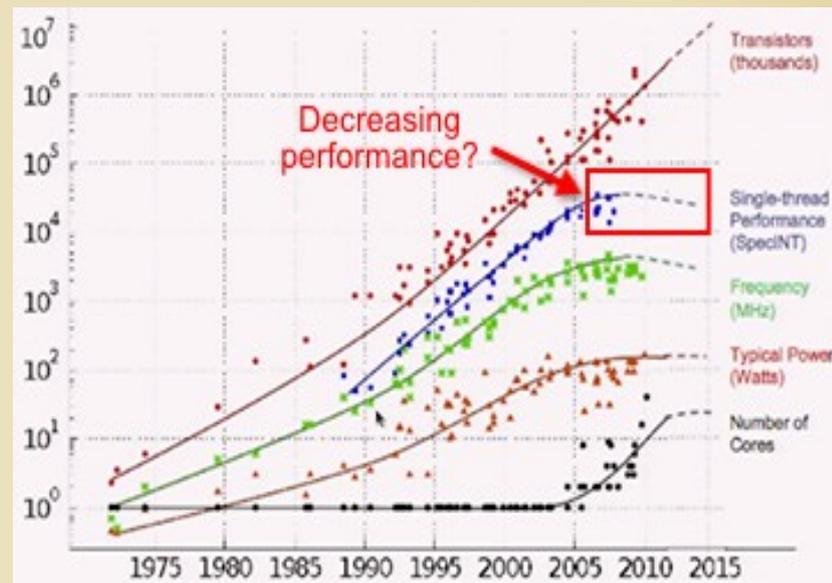


Fast computing=parallel computing

- Moore's law:



Every 2nd year the number of transistors (integrated circuits) are doubled in computing hardwares.

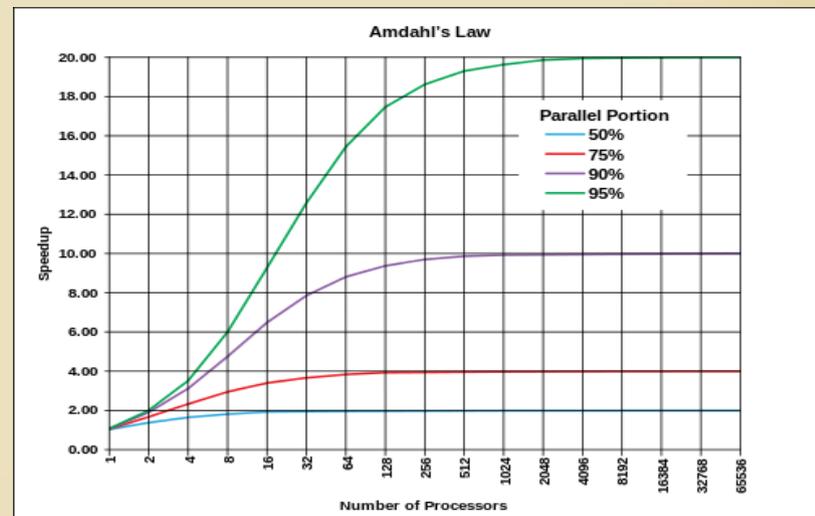


- Amdahl's law:



The theoretical speedup is given by the portion of parallelizable program, p , & number of processors, N , is:

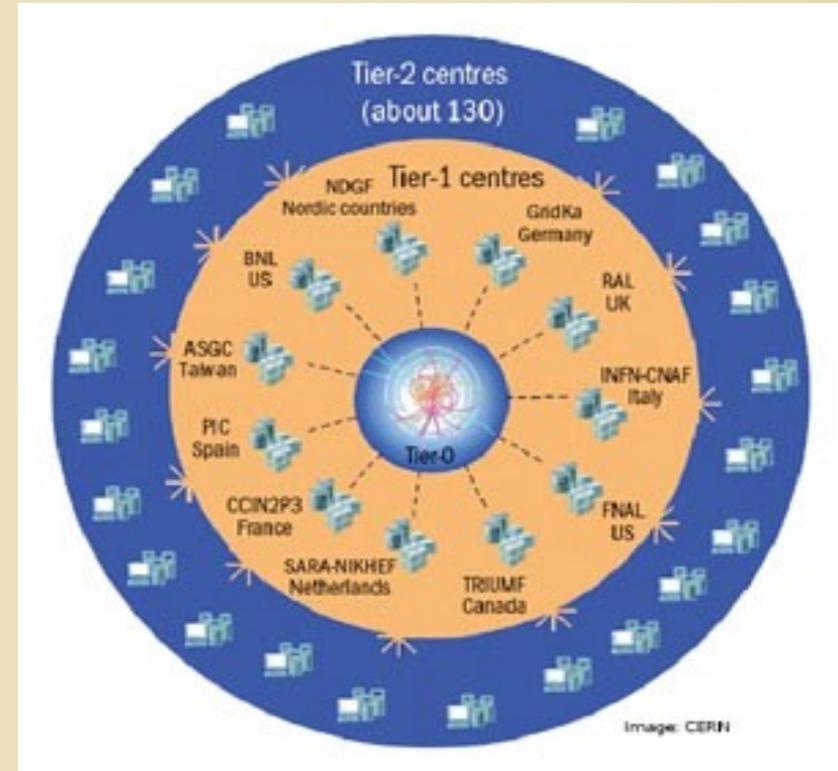
$$S(N) = \frac{1}{(1 - P) + \frac{P}{N}}$$



How to improve the WLCG resources

WLCG:

- Critical points are the number and performance of the WNs
- There are multicore machines with single thread.
- If there are free multicores or GPU resources, improvement can be made at the software and middleware level (cheap).
- Certainly, there is a budget issue as well.



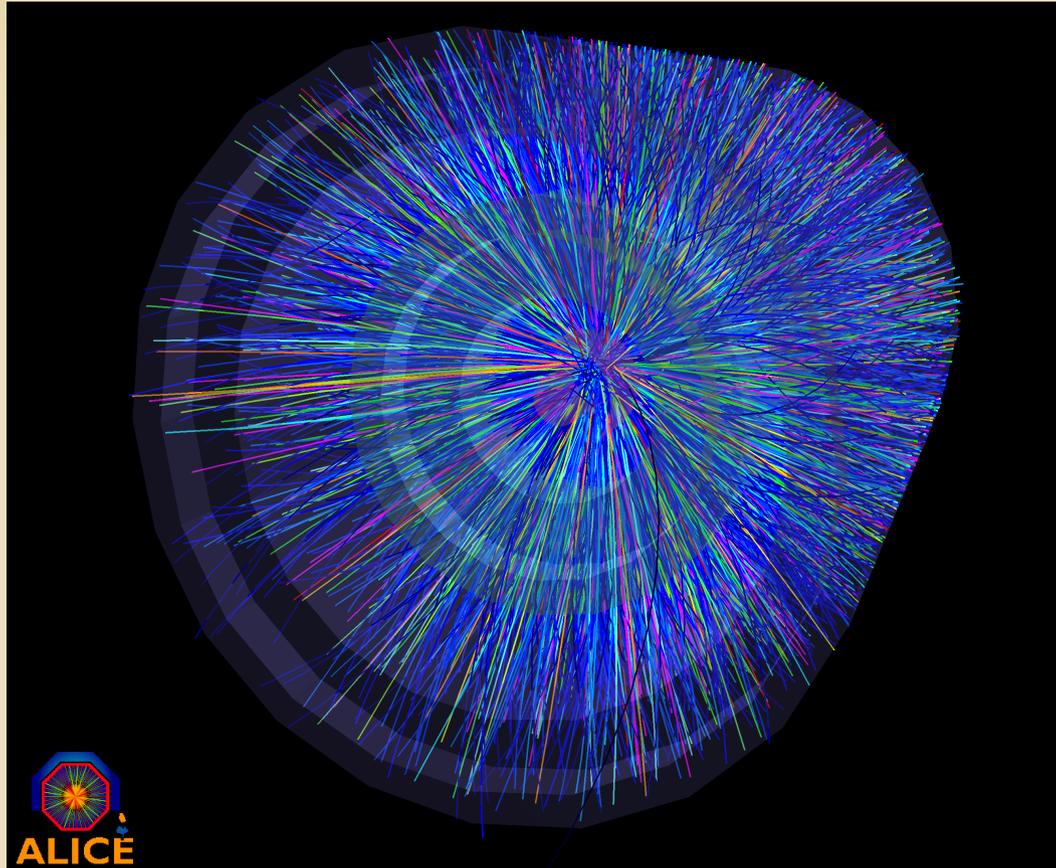
When is the moment to use GPUs?

No direct answer!

- Pilot study to define parameters to be optimized
- Need for large scale and large-large scale computing
- Have time (5-10 times more code development)
- Manpower high-level (close to hardware) programming
- \$\$\$\$\$

What has been done so far to help us? - without CUDA, etc...

- Several libs & toolkits (BLAS, FFTW, CUBLAS, CUFFT)
- Wrappers (C, FORTRAN → CUDA)
- OpenCL standards (Ati, NVidia)
- Mathematica, MatLab (with GPU support)



GPU based PRNG for MC event generators

GPU based PRNG for MC event generators

- Software frameworks

CERN

- OS: SLC 2.6.32-279.1.1.el6.x86_64
- Graphics: fglrx 9.002 (Catalyst 12.10)
- GCC: 4.4.6 20120305 (Red Hat 4.4.6-4)
- OpenCL: 1.2 AMD APP SDK 2.8

ALICE

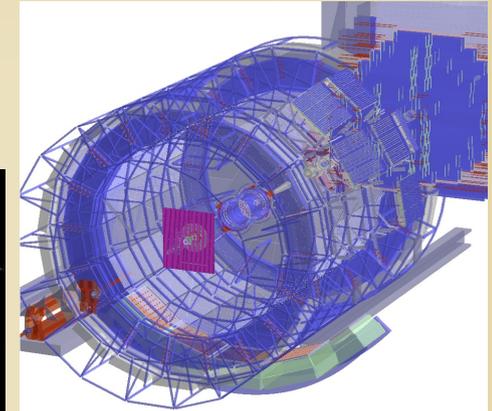
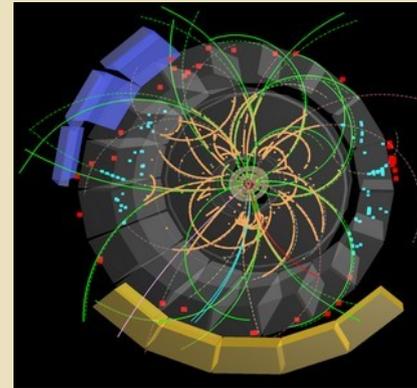
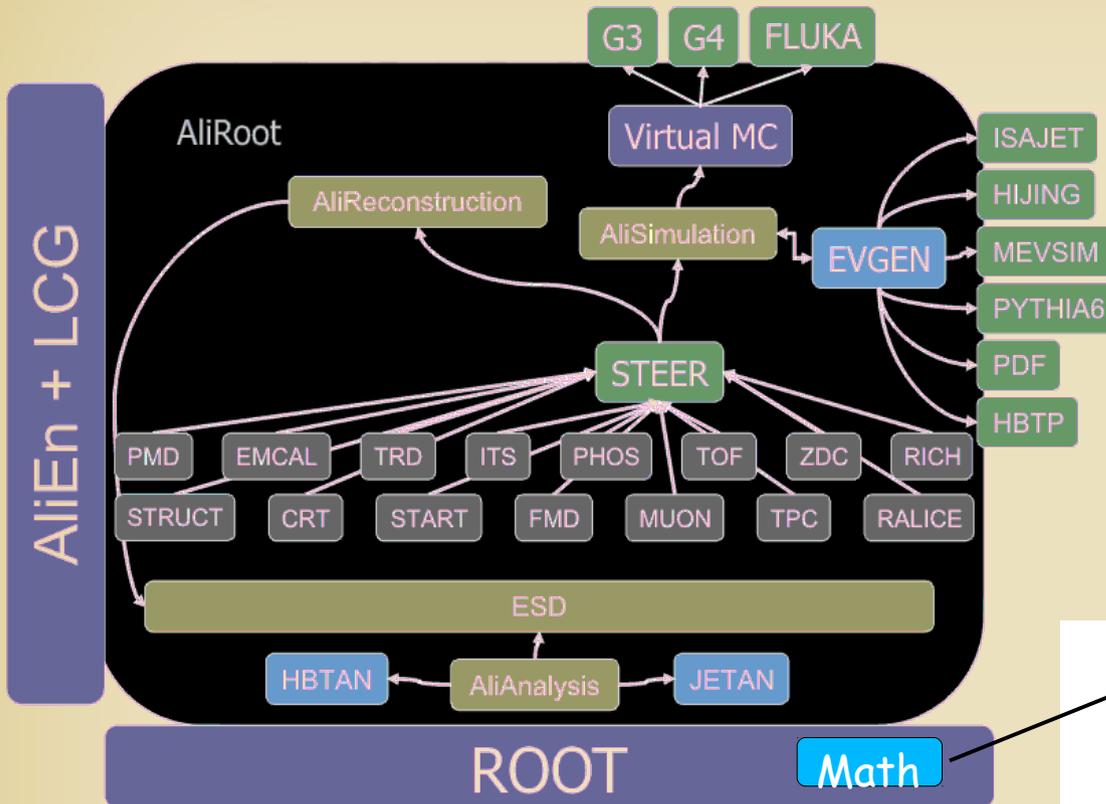
- Aliroot: v5-03-73-AN
- Root: v5-34-02
- Geant3: v1-14

PRNG tester

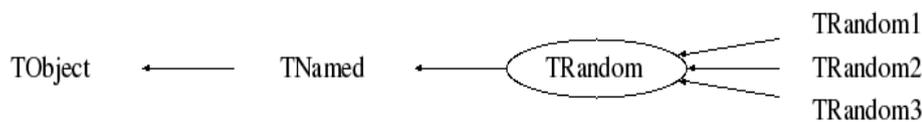
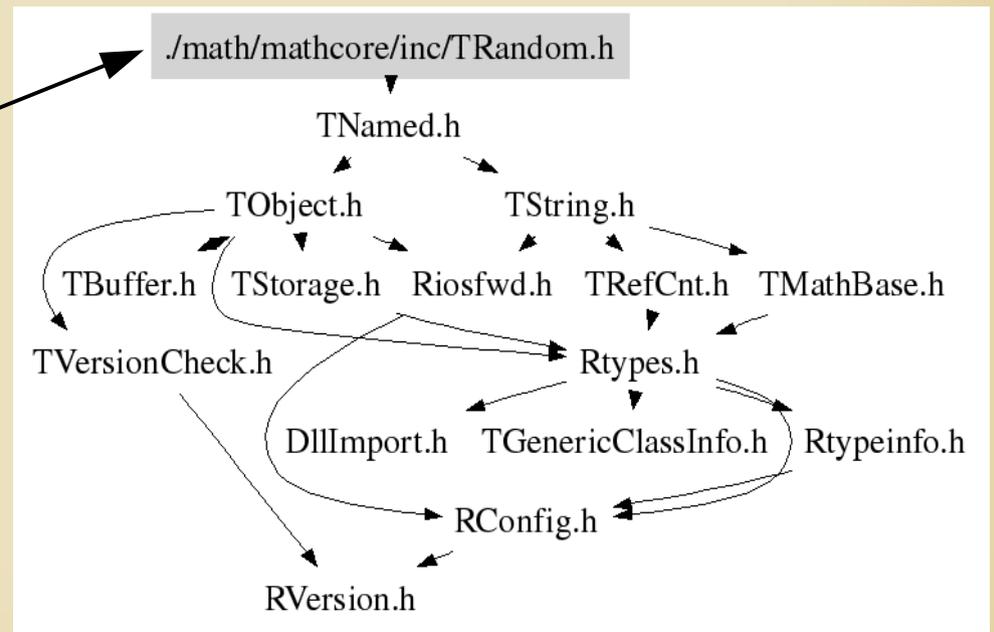
- Dieharder: 3.31.1



GPU based PRNG for MC event generators



AliRoot framework for ALICE data simulation, reconstruction, analysis



GPU based PRNG for MC event generators

- The tested PRNG codes

Trandom1 (RANLUX)

TRandom2 (Tausworthe)

TRandom3

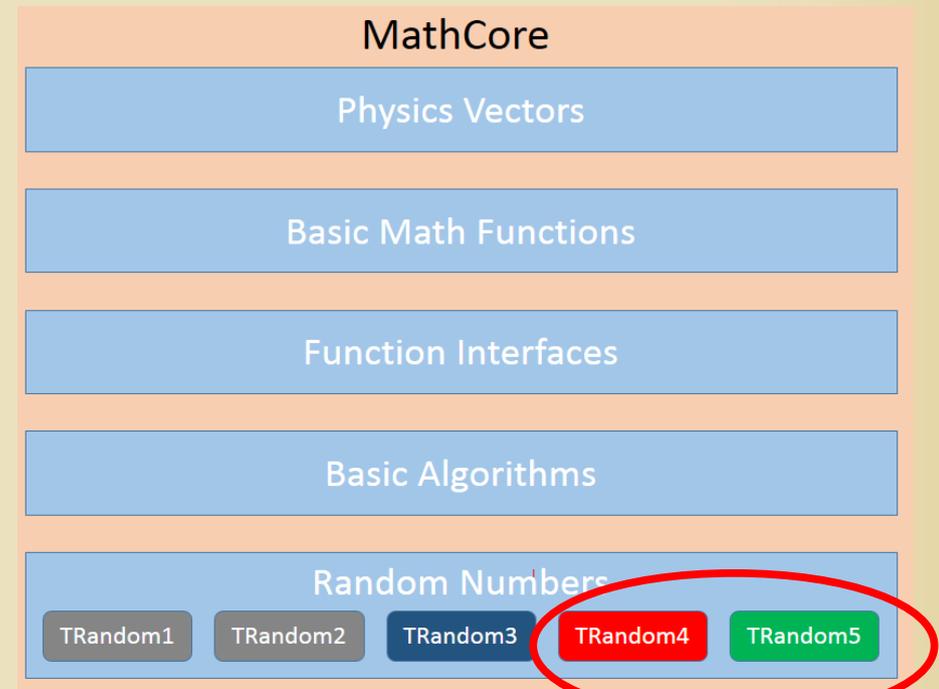
- Original CPU based Mersenne Twister) algorithm

TRandom4

- CPU/GPU based SFMT (SIMD-oriented Fast Mersenne Twister) algorithm

TRandom5

- CPU/GPU based MWC64X algorithm



GPU based PRNG for MC event generators

- From the *user side*

- Installation:

 - Driver + OpenCL (SDK)

 - Pre-compiled modules

- Usage:

 - TRandomX, can be take as a regular PRNG.

 - CPU/GPU run can be choosen via parameters:

 - GPU: parameter > 200

 - CPU: parameter < 200

```
AliGenerator* CreateGenerator();

//void fastGen(Int_t nev = 50000, char* filename = "galice.root")
void fastGen(Int_t nev = 20000, char* filename = "galice.root")
{
  // Runloader
  TStopwatch timer;
  timer.Start();
  gSystem->SetIncludePath("-I$ROOTSYS/include -I$ALICE_ROOT/include -I$ALICE_ROOT");
  gSystem->Load("liblhpdf.so"); // Parton density functions
  gSystem->Load("libEGPythia6.so"); // TGenerator interface
  gSystem->Load("libpythia6.so"); // Pythia
  gSystem->Load("libAliPythia6.so"); // ALICE specific implementations

  AliRunLoader* r1 = AliRunLoader::Open("galice.root","FASTRUN","recreate");

  r1->SetCompressionLevel(2);
  r1->SetNumberOfEventsPerFile(nev);
  r1->LoadKinematics("RECREATE");
  r1->MakeTree("E");
  gAlice->SetRunLoader(r1);

  // Create stack
  r1->MakeStack();
  AliStack* stack = r1->Stack();

  // Header
  AliHeader* header = r1->GetHeader();

  // Setting TRandom4 as default generator
  TRandom5 r5(201);
  gRandom=&r5;

  // Create and Initialize Generator
  AliGenerator *gener = CreateGenerator();
  gener->Init();
  gener->SetStack(stack);
}
```

GPU based PRNG for MC event generators

- Behind the scene

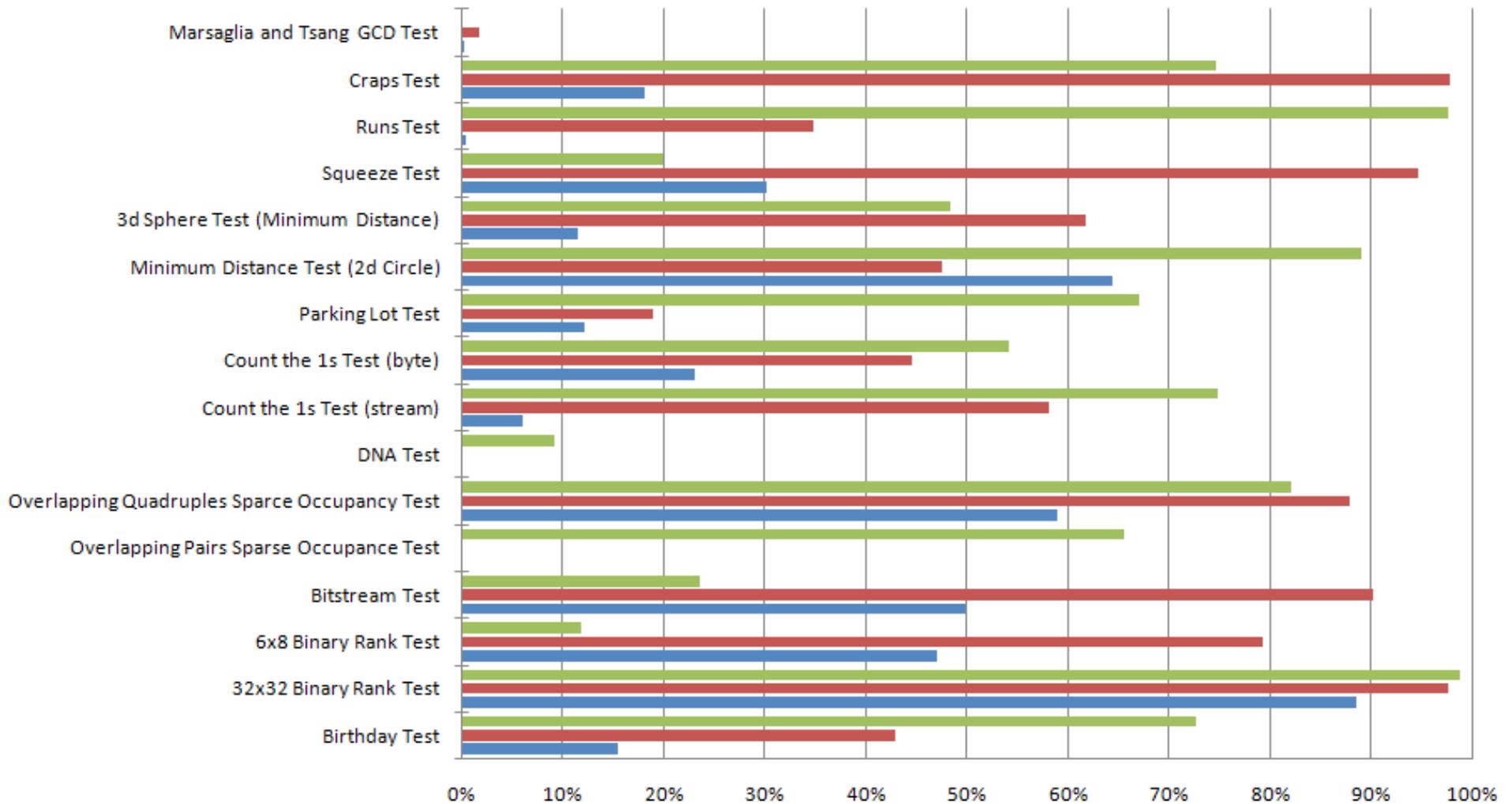
- TRandom4 & TRandom5
- No single random number generation only in 500k blocks
- RAM buffer is for random numbers.
- Only speeddown is the 'stack depth check'.
- Copy work from buffer is by the CPU.
- Due to OpenCL platform this works on both CPU/GPU

- Constructor

- It contains all tasks
 - Platform check
 - Context creation
 - Device info
 - Kernel compilation
 - Command queue
 - Buffer allocation
 - Sending random seeds to devices
 - Tread ID settings

The PRNG quality test

Results of Dieharder Tests



TRandom3 TRandom4 TRandom5

The PRNG quality test

- Summary of the DieHard quality tests of PRNGs

TRandom3 - Original CPU based Mersenne Twister

TRandom4 - CPU/GPU based SFMT (SIMD-oriented Fast MT)

TRandom5 - CPU/GPU based MWC64X algorithm

PRNG modules	Platform	Total Kuiper KS p
TRandom3	CPU	29.27 %
TRandom4	CPU/GPU	53.59 %
TRandom5	CPU/GPU	55.56 %

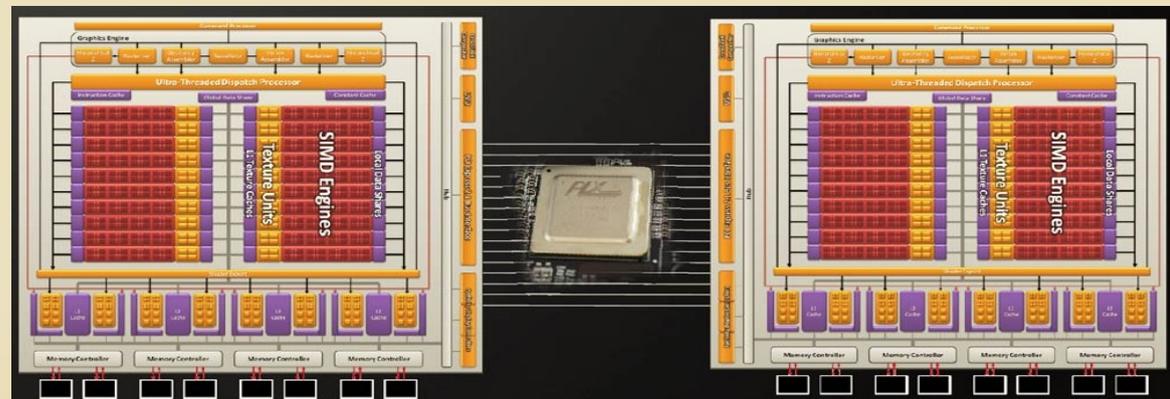
Performance ↓

Performance tests by GPU based MC

- Hardware framework

gpu001 at GPU Laboratory of the Wigner RCP

- MB: ASUS P6T6 PCIExpress 2.0x16
- CPU: Core i7 920 (2.76 Ghz, 8 KB cache)
- Memory: 12GB DDR3 (1333 MHz)
- HDD: 1 TB
- GPU: 3 pcs. ATi Radeon HD5970
(2 GPUs, 735 MHz, 1+1 GB GDDR, 4.64 TFlop)



Performance tests by GPU based MC

- Hardware framework

gpu001 at GPU Laboratory of the Wigner RCP



The main question is: How about SPEED?

- Levels of speedtest

Kernel speed

- Real generation time of a PRNG in CPU or in GPU.

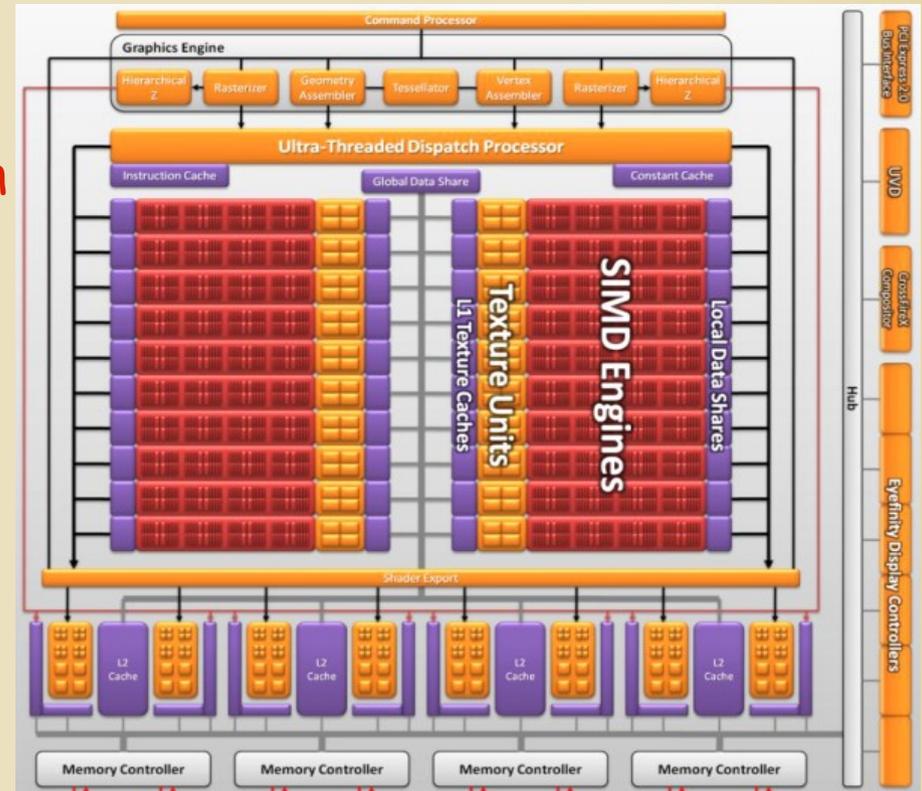
Total speed

- Generation time of the PRNGs within the proper program framework

Real speed

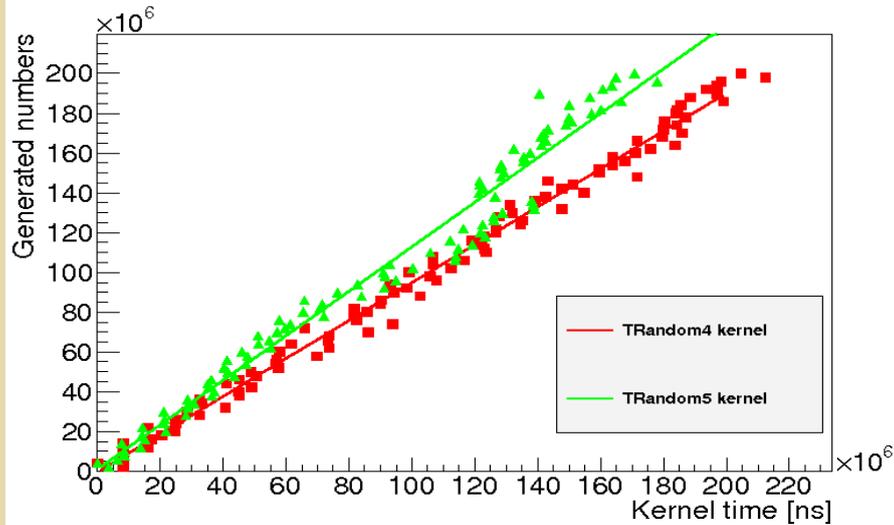
- The above two, but with real (V)RAM usage.

Here we used a 200 million event sample!

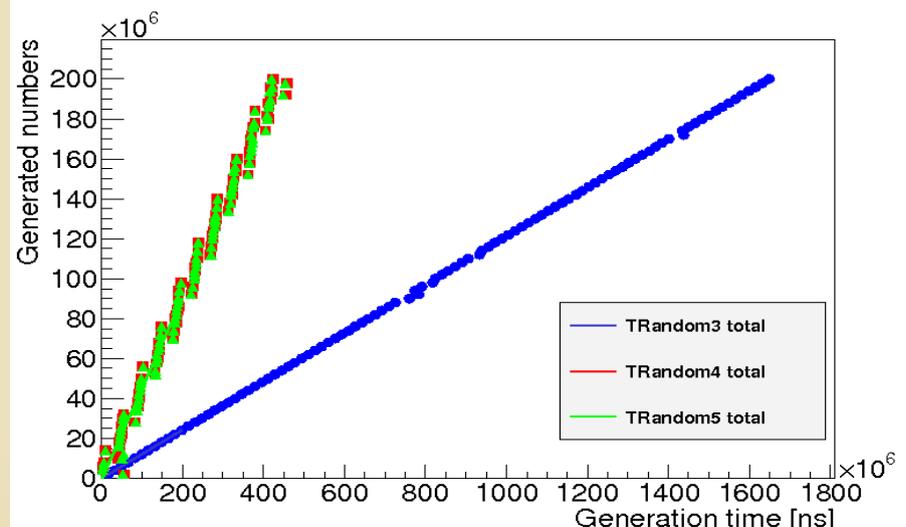
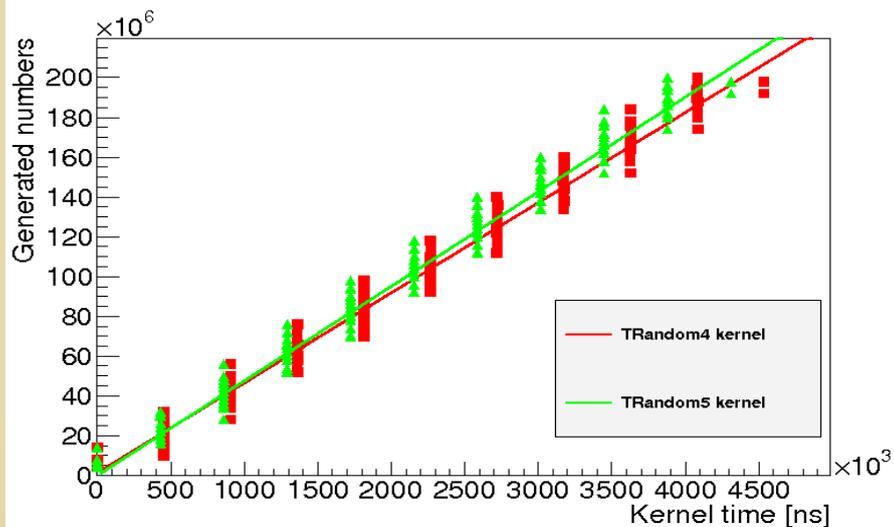
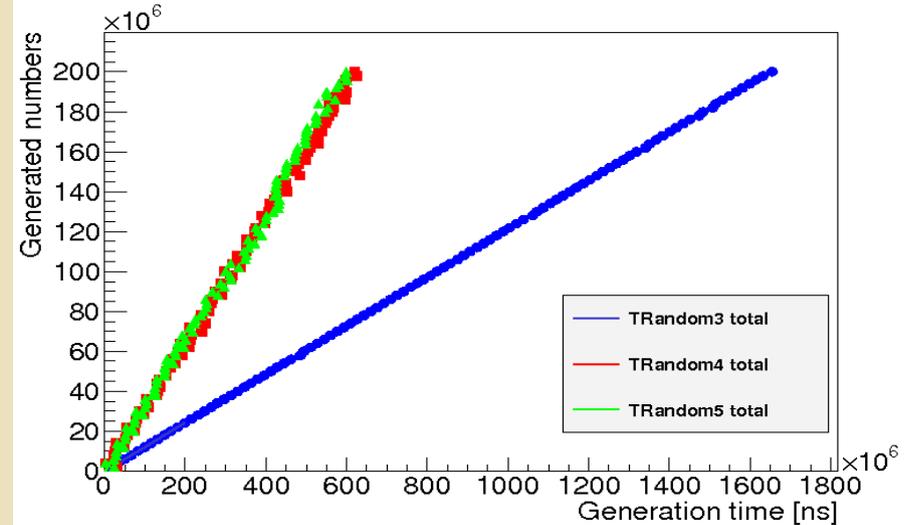


SPEED without writing (V)RAM

Kernel time



Full calculation

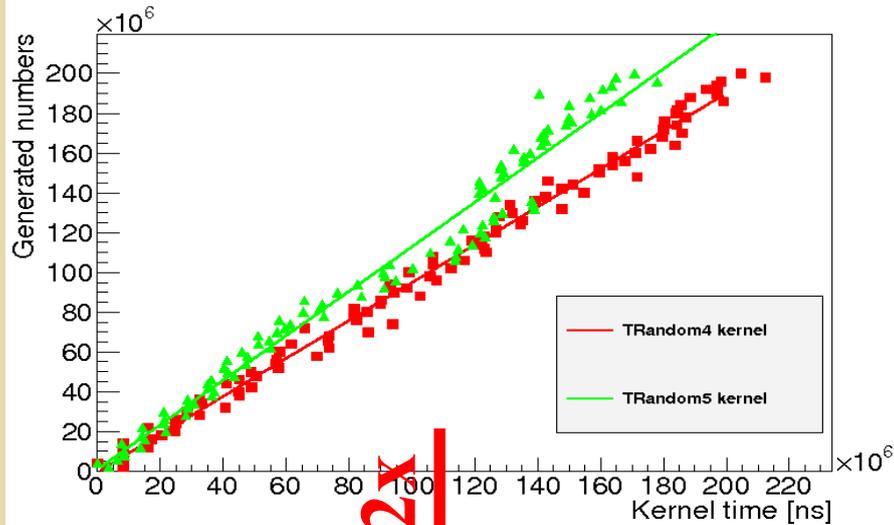


CPU

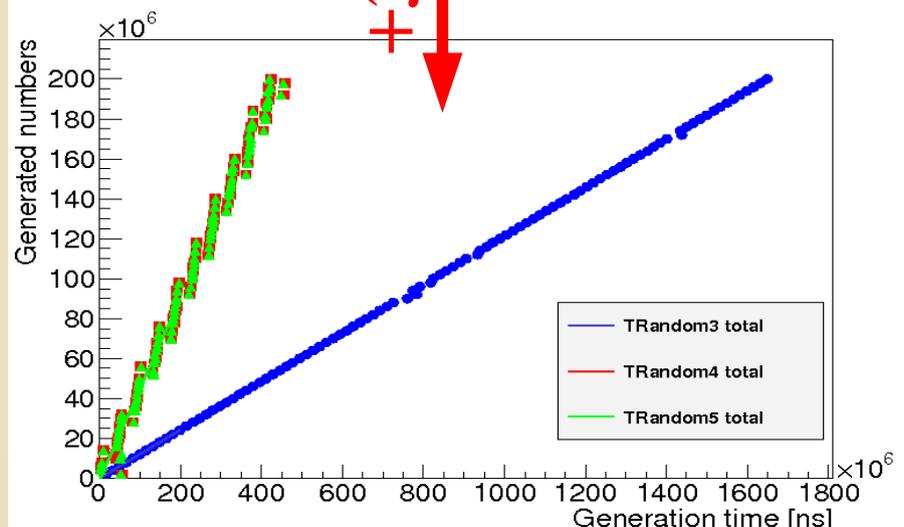
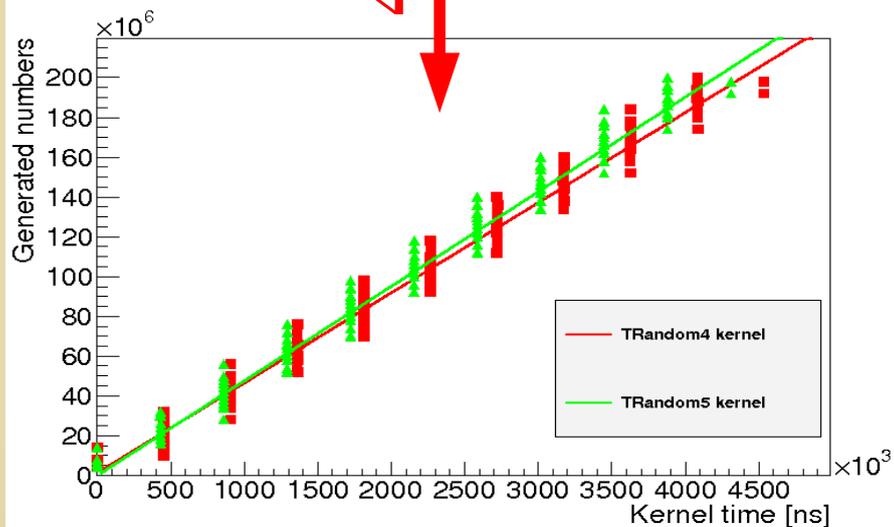
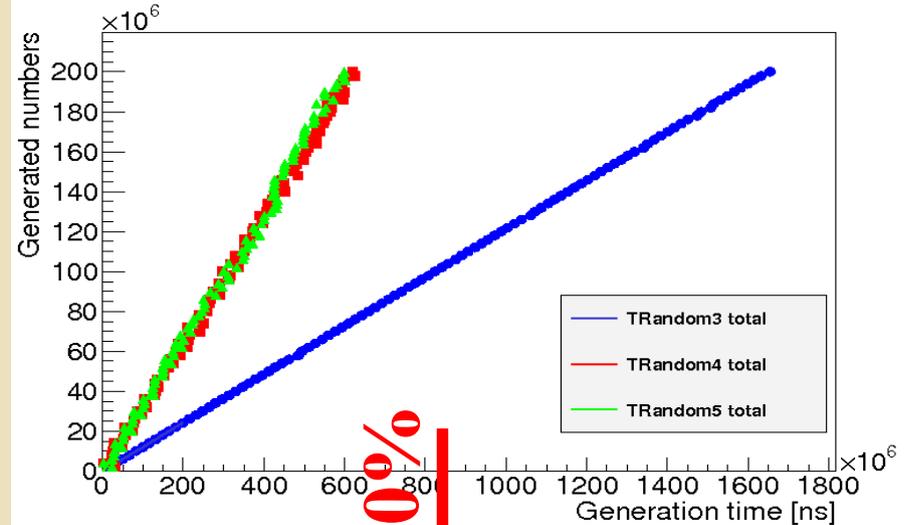
GPU

SPEED without writing (V)RAM

Kernel time



Full calculation

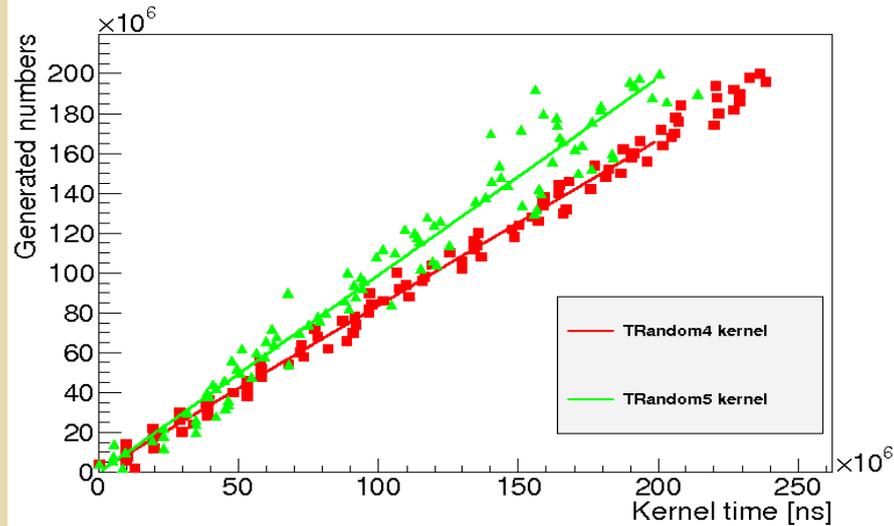


CPU

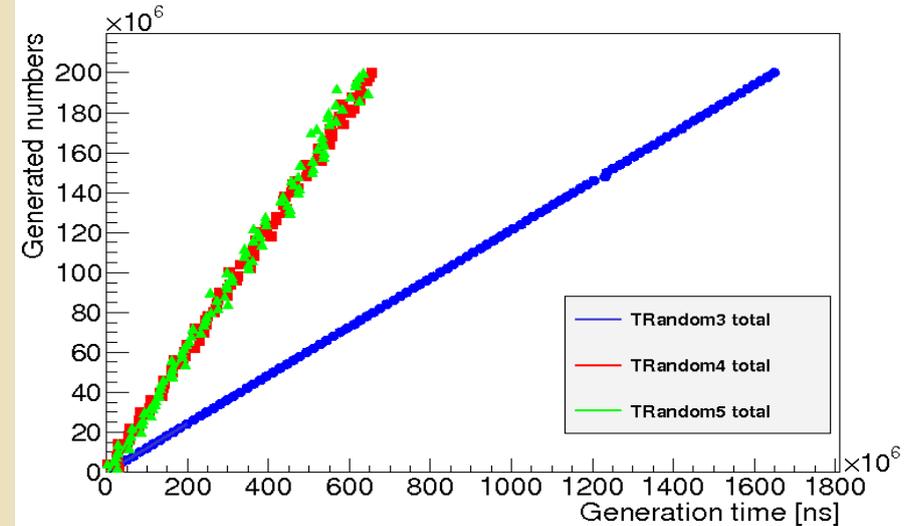
GPU

SPEED with writing (V)RAM

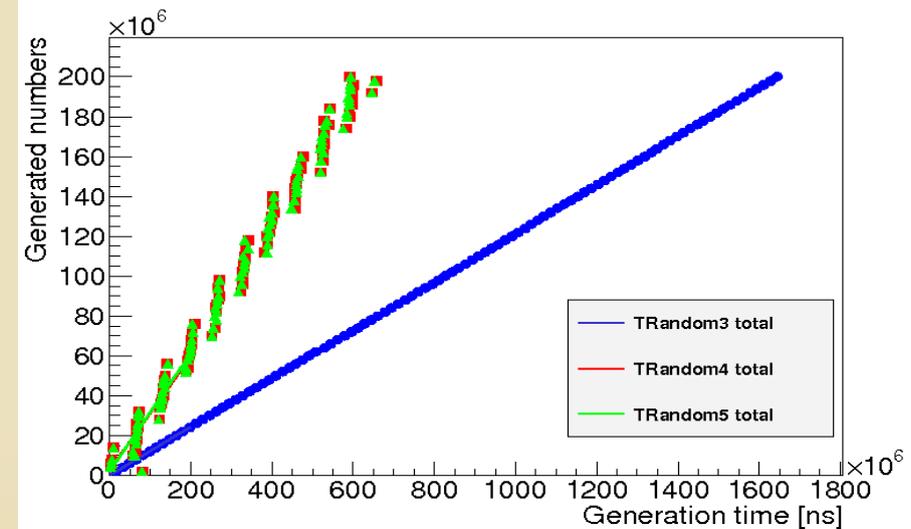
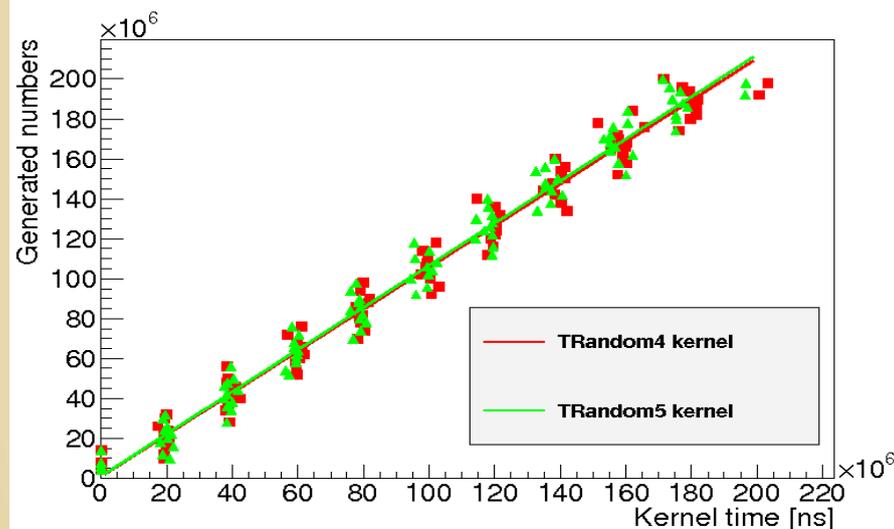
Kernel time



Full calculation



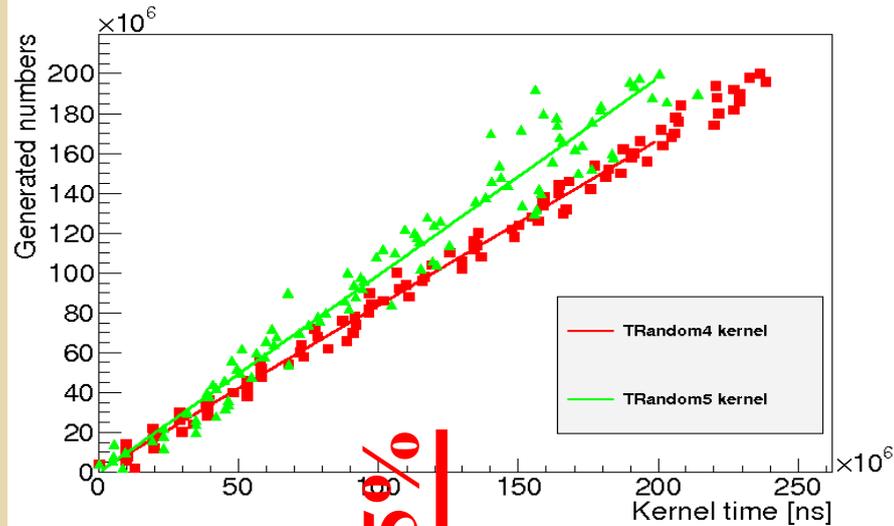
CPU



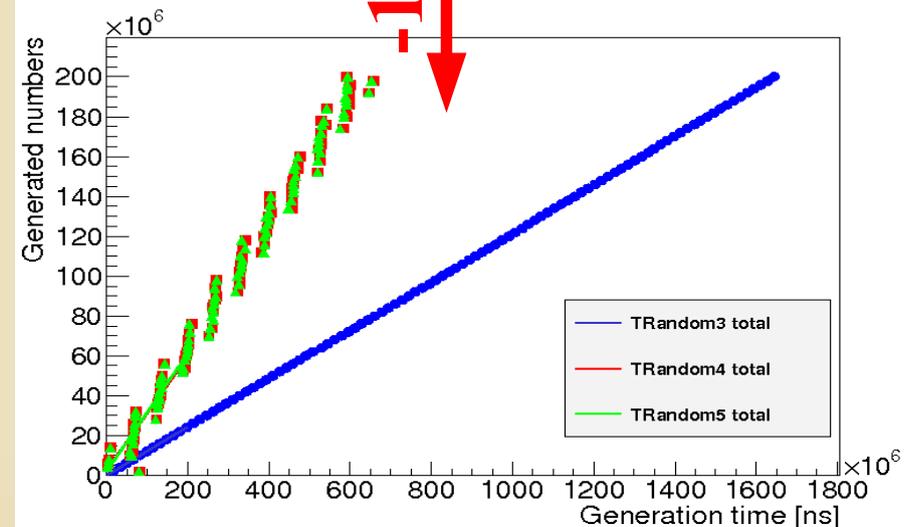
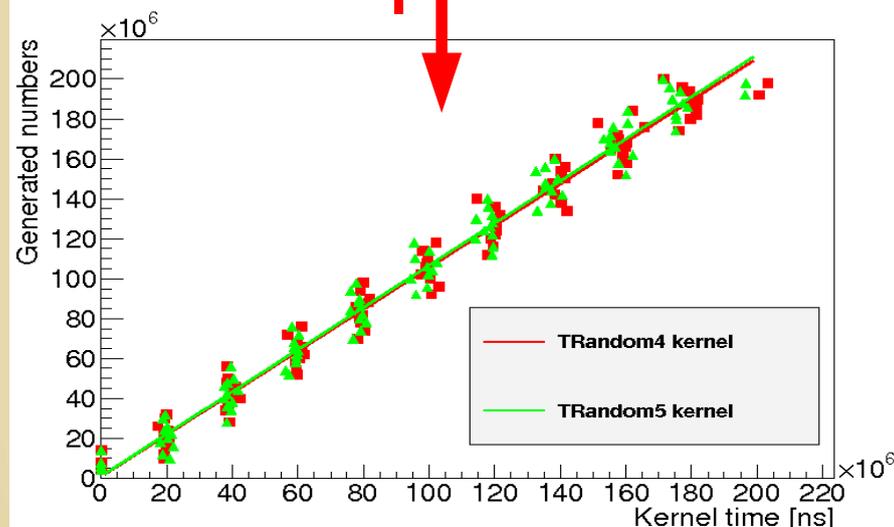
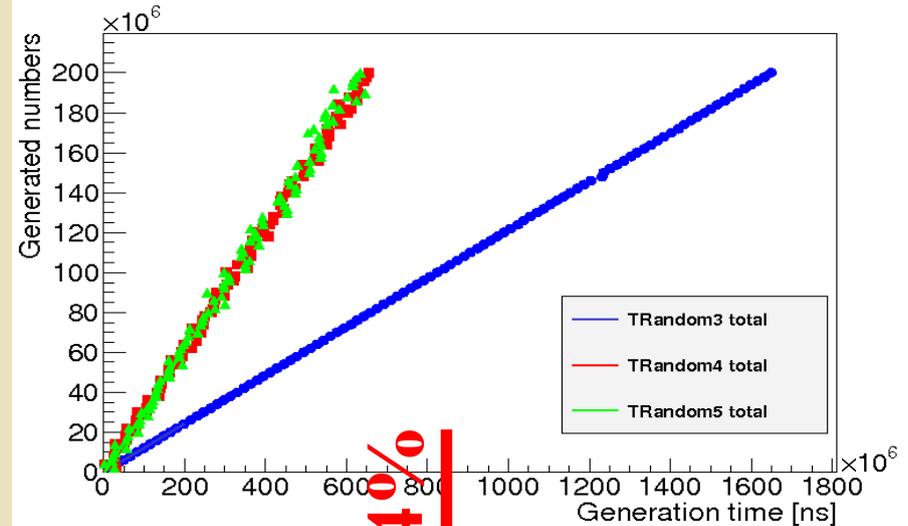
GPU

SPEED with writing (V)RAM

Kernel time



Full calculation



CPU

GPU

So, how about SPEED test?

- For this setup (Core i7 vs. ATi Radeon HD5970)

TRandom3 < TRandom4 < Trandom5

PRNG modules and run types	VCPU kernel [#/ μ s]	VGPU kernel [#/ μ s]	VCPU total [#/ μ s]	VGPU total [#/ μ s]
TRandom3 RW	121.71 \pm 0.22%	—	121.71 \pm 0.22%	—
TRandom4 RW	953.44 \pm 0.96%	1047.22 \pm 1.59%	321.38 \pm 2.94%	284.846 \pm 7.89%
TRandom5 RW	1 118.87 \pm 1.72%	1055.64 \pm 1.58%	338.06 \pm 2.50%	295.71 \pm 6.76%
TRandom3 NW	121.69 \pm 0.15%	—	121.69 \pm 0.15%	—
TRandom4 NW	953.44 \pm 0.96%	45 325.54 \pm 2.23%	321.379 \pm 2.94%	451.910 \pm 3.51%
TRandom5 NW	1 118.87 \pm 1.72%	47 583, 52 \pm 3.16%	338.059 \pm 2.50%	456.508 \pm 3.62%

Annotations: Red arrows on the left indicate a +10x speedup from RW to NW for TRandom3 and TRandom5. Red arrows on the right indicate a +3x speedup for TRandom4 and TRandom5 when comparing VCPU total to VGPU total.

So, how about SPEED test?

- For this setup (Core i7 vs. ATi Radeon HD5970)

TRandom3 < TRandom4 < Trandom5

Kernel calculation is faster (NW)

PRNG modules and run types	VCPU kernel [#/ μ s]	VGPU kernel [#/ μ s]	VCPU total [#/ μ s]	VGPU total [#/ μ s]
TRandom3 RW	121.71 \pm 0.22%	—	121.71 \pm 0.22%	—
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So, how about SPEED test?

- For this setup (Core i7 vs. ATi Radeon HD5970)

TRandom3 < TRandom4 < Trandom5

Kernel calculation is faster (NW), but real speed (RW) is slower

PRNG modules and run types	VCPU kernel [#/ μ s]	VGPU kernel [#/ μ s]	VCPU total [#/ μ s]	VGPU total [#/ μ s]
TRandom3 RW	121.71 \pm 0.22%	—	121.71 \pm 0.22%	—
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Annotations: +10x (vertical arrows on left), +3x (vertical arrows on right), -5% (horizontal arrow between VCPU and VGPU kernel for RW), -14% (horizontal arrow between VCPU and VGPU total for RW), +45x (horizontal arrow between VCPU and VGPU kernel for NW), +30% (horizontal arrow between VCPU and VGPU total for NW).

Note₁: New GPU cards are 2-5 times faster

So, how about SPEED test?

- For this setup (Core i7 vs. ATi Radeon HD5970)

TRandom3 < TRandom4 < Trandom5

Kernel calculation is faster (NW), but real speed is slower

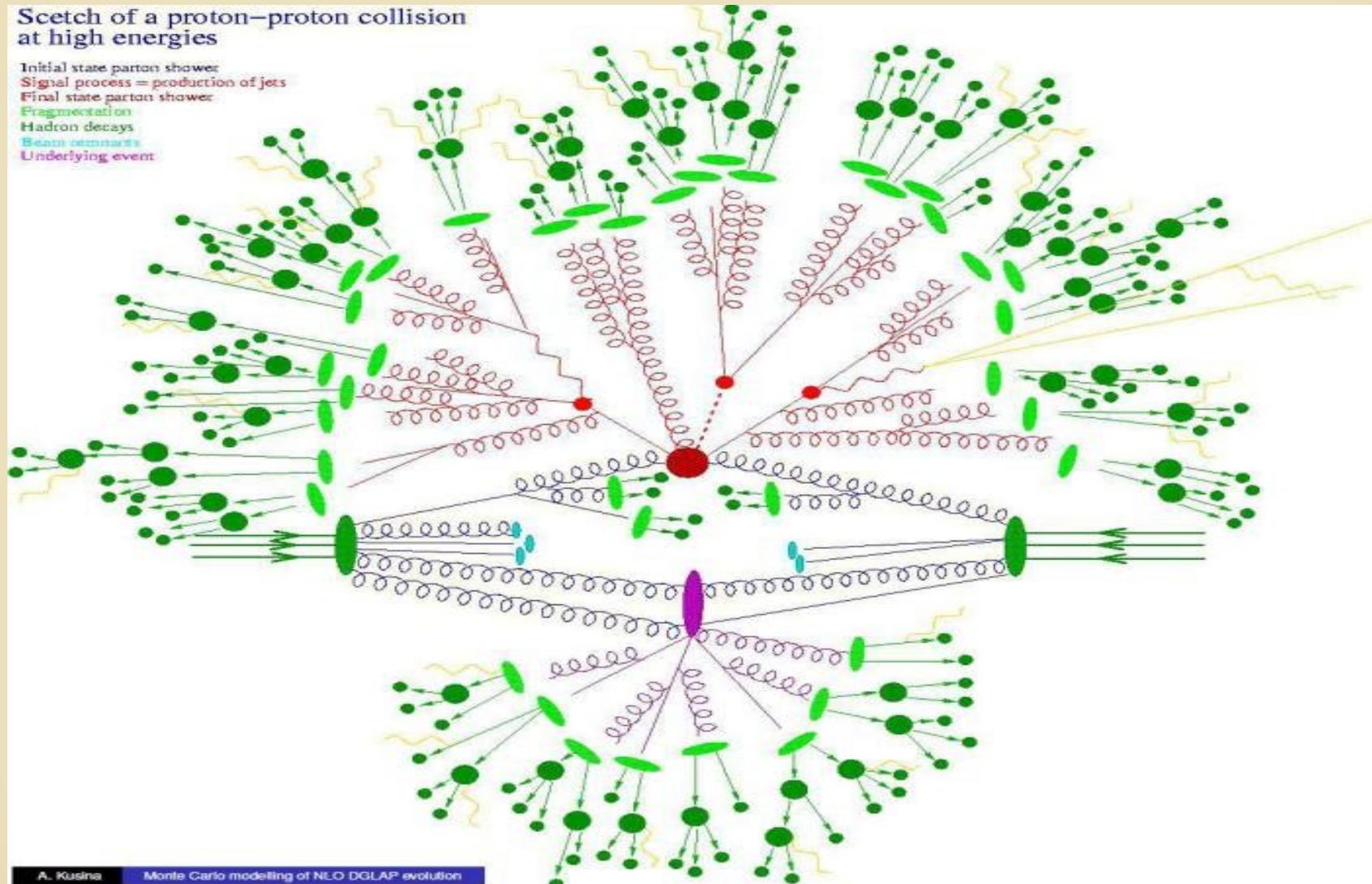
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#2x faster

Note₂: Parallel computing (OpenCL) improves speed!

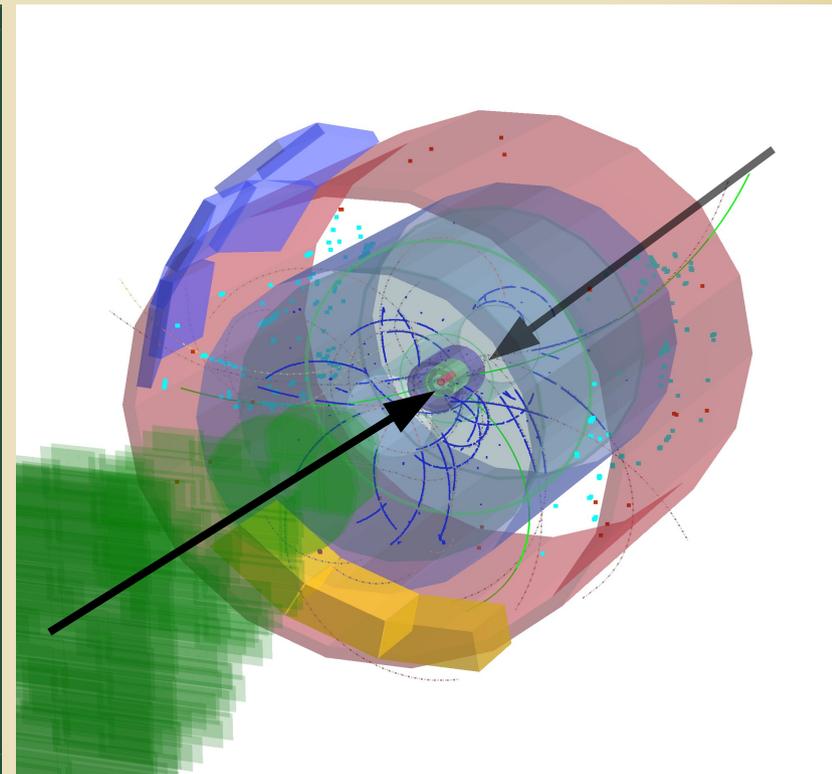
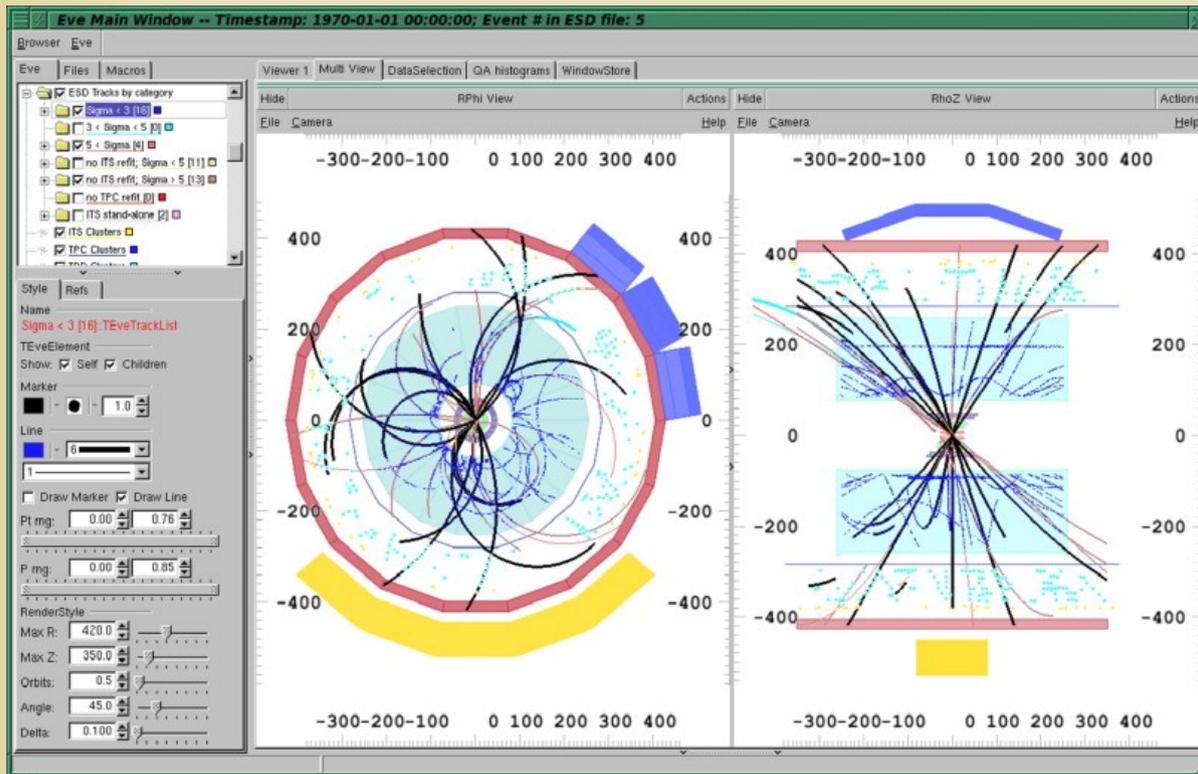
Some Physics: proton-proton collisions

- Theoretical model of a pp collisions



Some Physics: proton-proton collisions

- A reconstructed pp event in the ALICE experiment

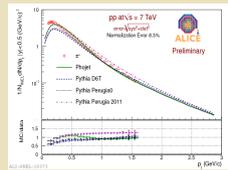


Some Physics: pp collisions at GPU

- 400k TRandom5 PRNG

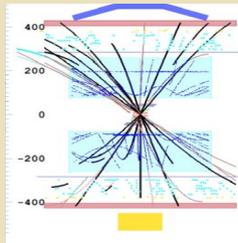
Transverse momentum spectrum

dN/dp_T (Tsallis distr.)



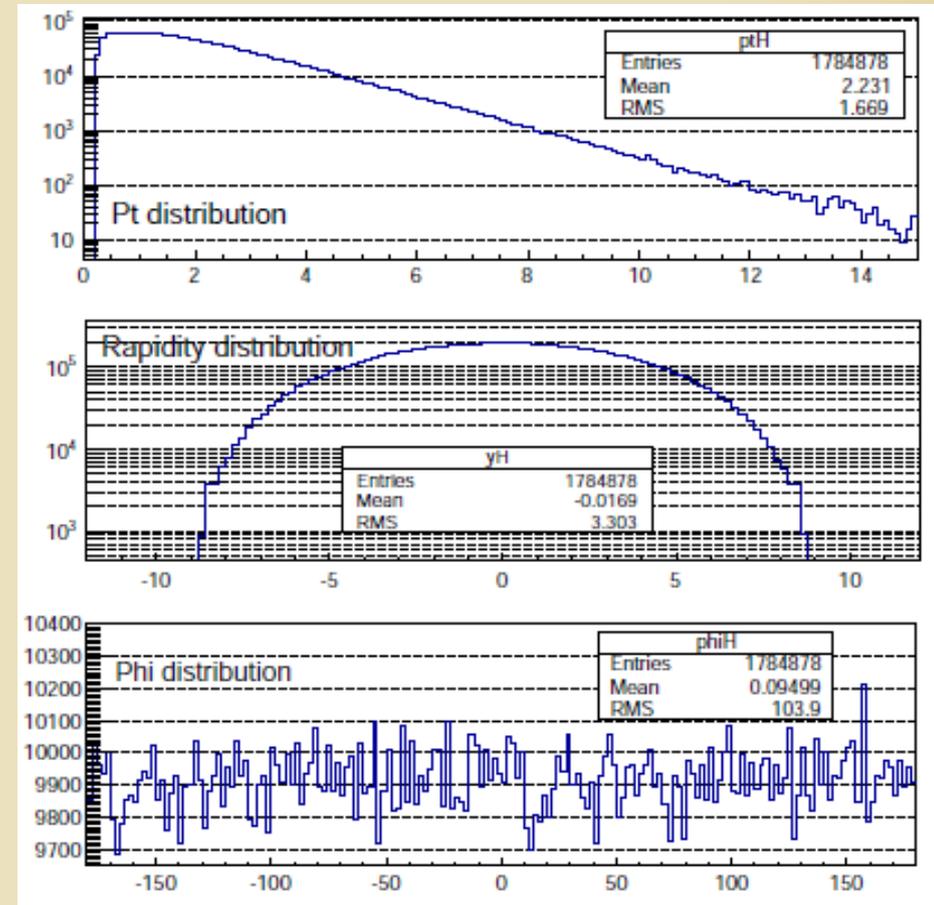
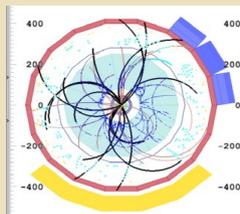
Rapidity distribution

dN/dy (Gaussian distr.)



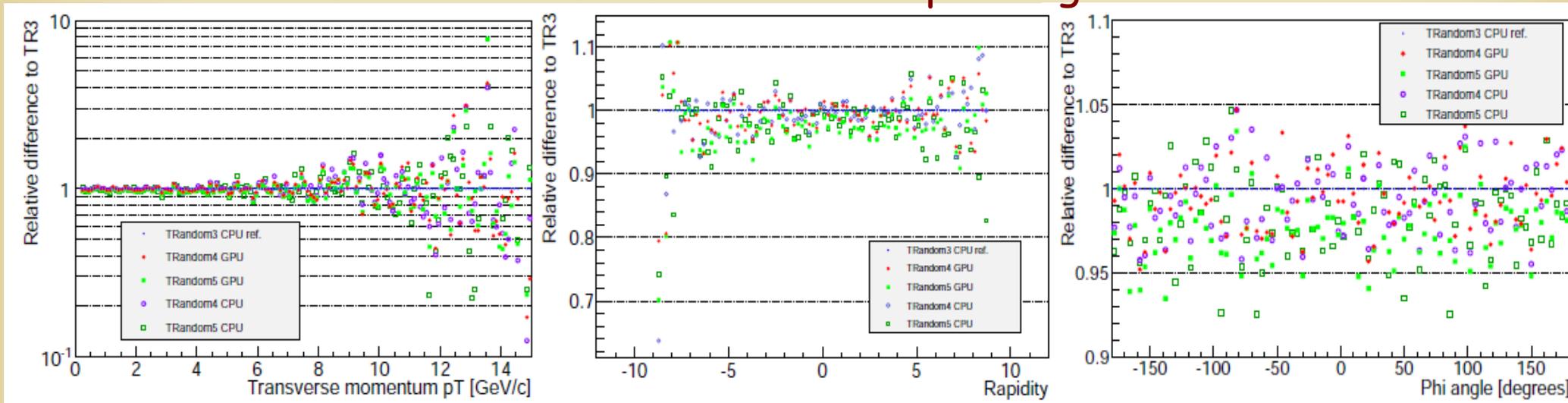
Angular distribution

$dN/d\phi$ (Isotropy)



Some Physics: pp collisions at GPU

- To check the validity of the 'physics':
 - Compare calculated distributions to the original Trandom3 CPU
 - $\text{TRandomX}/\text{TRandom3}$ must be ~ 1 depending on statistics

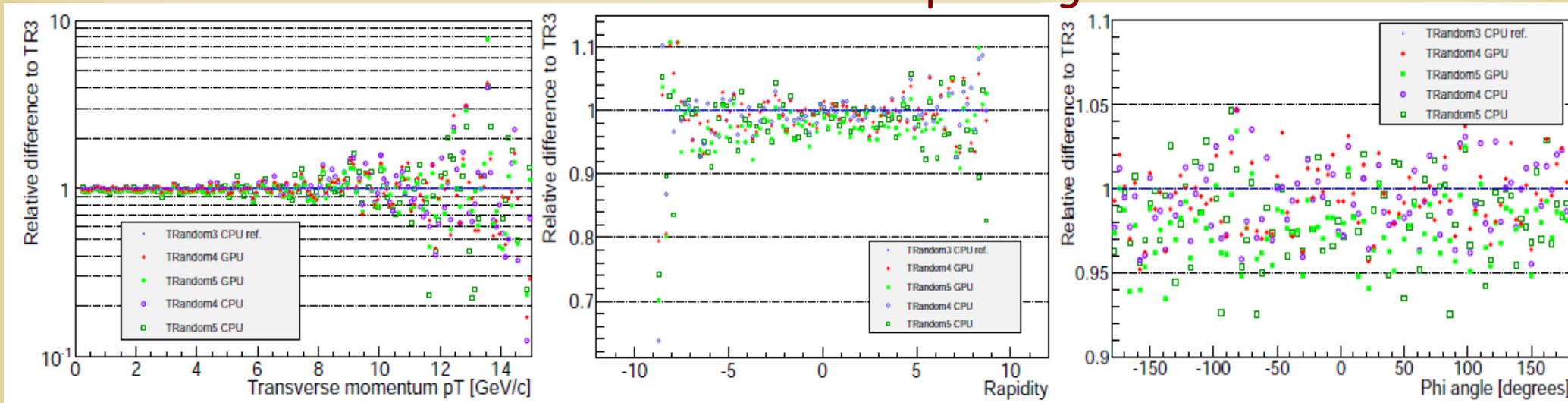


Some Physics: pp collisions at GPU

- To check the validity of the 'physics':

Compare calculated distributions to the original Trandom3 CPU

$\text{TRandomX}/\text{TRandom3}$ must be ~ 1 depending on statistics



10% agreement
up to $p_T < 6 \text{ GeV}/c$

5% agreement
in $|y| < 5$

5% agreement
in the whole ϕ

S U M M A R Y

- Aim
 - Faster MC event generation for HIC
- Results for pp MC @ GPUs
 - Diehard test of open source PRNGs: (SFMT, MWC64X) on GPUs
 - Implementation of new GPU based modules (TRandom4, TRandom5) to Root/AlRoot framework
 - Tests: simulation of high-energy pp collisions
- Take away message
 - GPUs can be used for Monte Carlo generators in HIC
 - One needs more programming (CUDA/OpenCL/...)
 - Need to optimize (price/speed) since other technologies available (e.g. Intel Xeon Phi)

OUTLOOK

- The presented results are on
 - AliRoot, especially AliPYTHIA for proton-proton
 - CPU/GPU SIMD-oriented Fast MT & MWC64X
 - Standalone machine (with ATi Radeon HD5970)
- How to improve?
 - Ongoing: HIJING calculations (need for more PRNGs), so might be more efficient, faster
 - Trivial: Buy new fast cards and re-test - we are on it and we hope the funding agency on it as well.
 - The framework is almost ready to test in the GRID using JDL (required HW: GPUs, SW: OpenCL/CUDA/...)
 - More faster PRNGs on CPUs/GPUs (Tiny MT, MTGP), but note, faster PRNG less randomness quality.
 - Further modules can be moved to GPU

BACKUP

The PRNG quality test

Some DieHard tests by George Marsaglia

Birthday spacings: Choose random points on a large interval. The spacings between the points should be asymptotically exponentially distributed. The name is based on the birthday paradox.

Overlapping permutations: Analyze sequences of five consecutive random numbers. The 120 possible orderings should occur with statistically equal probability.

Ranks of matrices: Select some number of bits from some number of random numbers to form a matrix over $\{0,1\}$, then determine the rank of the matrix. Count the ranks.

Monkey tests: Treat sequences of some number of bits as "words". Count the overlapping words in a stream. The number of "words" that don't appear should follow a known distribution. The name is based on the infinite monkey theorem.

Count the 1s: Count the 1 bits in each of either successive or chosen bytes. Convert the counts to "letters", and count the occurrences of five-letter "words".

Parking lot test: Randomly place unit circles in a 100×100 square. If the circle overlaps an existing one, try again. After 12,000 tries, the number of successfully "parked" circles should follow a certain normal distribution.

Minimum distance test: Randomly place 8,000 points in a $10,000 \times 10,000$ square, then find the minimum distance between the pairs. The square of this distance should be exponentially distributed with a certain mean.

Random spheres test: Randomly choose 4,000 points in a cube of edge 1,000. Center a sphere on each point, whose radius is the minimum distance to another point. The smallest sphere's volume should be exponentially distributed with a certain mean.

The squeeze test: Multiply 231 by random floats on $[0,1)$ until you reach 1. Repeat this 100,000 times. The number of floats needed to reach 1 should follow a certain distribution.

Overlapping sums test: Generate a long sequence of random floats on $[0,1)$. Add sequences of 100 consecutive floats. The sums should be normally distributed with characteristic mean and sigma.

Runs test: Generate a long sequence of random floats on $[0,1)$. Count ascending and descending runs. The counts should follow a certain distribution.

The craps test: Play 200,000 games of craps, counting the wins and the number of throws per game. Each count should follow a certain