



Design and Implementation of Vectorized Pseudorandom Number Generators

Master's Thesis Defense and Presentation

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Outline

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Pseudorandom Number Generators

Design of the Library

Vectorization and SIMD Architectures

Implementation of the Xoroshiro128+

Implementation of the MT19937

Implementation of Uniform Distribution Functions

Evaluation and Results

Conclusions and Future Work

Introduction

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What do we need random numbers for?

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- ▶ Physical Simulations, based on Monte-Carlo Methods

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- ▶ create a software library with powerful API
- ▶ compare performance to others implementations
- ▶ apply library to physical problems

Pseudorandom Number Generators

True Randomness

What is a random sequence?

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- ▶ existing formal concepts not applicable to computer systems

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- ▶ Unreproducibility

True Randomness

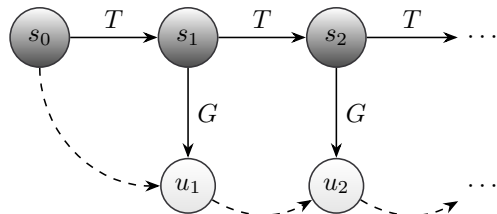
What is a random sequence?

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Disadvantages:

- ▶ Unreproducibility
- ▶ Speed Limitations

Pseudorandom Number Generator Definition



$S \dots$ Set of States

$T \dots$ Transition Function

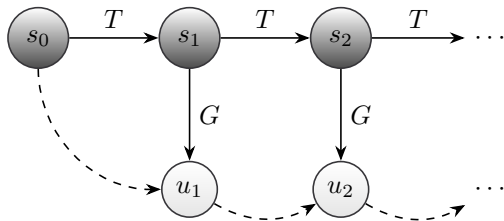
$U \dots$ Set of Possible Outputs

$G \dots$ Generator Function

$$\mathcal{G} := (S, T, U, G), \quad T: S \rightarrow S, \quad G: S \rightarrow U$$

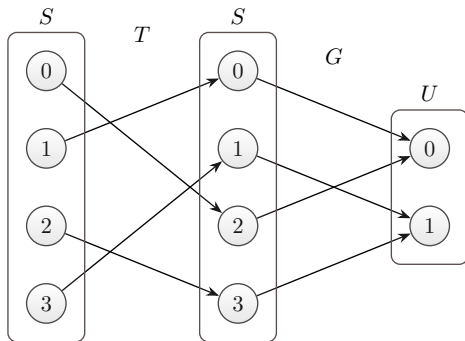
$$s_0 \in S, \quad s_{n+1} := T(s_n), \quad u_n := G(s_n)$$

Pseudorandom Number Generator Concept



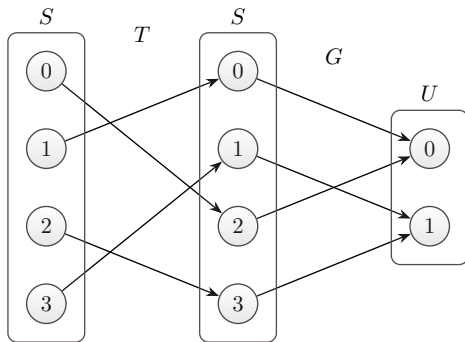
$$s_0 \sim \mathcal{U}_S, \quad u_1 \leftarrow \mathcal{G}(), \quad u_2 \leftarrow \mathcal{G}(), \quad u_3 \leftarrow \mathcal{G}(), \quad \dots$$

Pseudorandom Number Generator Example



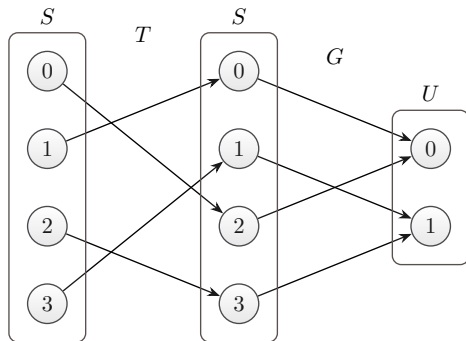
$$s_0 := 0, \quad (s_n) = \overline{2310}, \quad (u_n) = \overline{0110}$$

Pseudorandom Number Generator Example



- construction of “good” PRNG is difficult

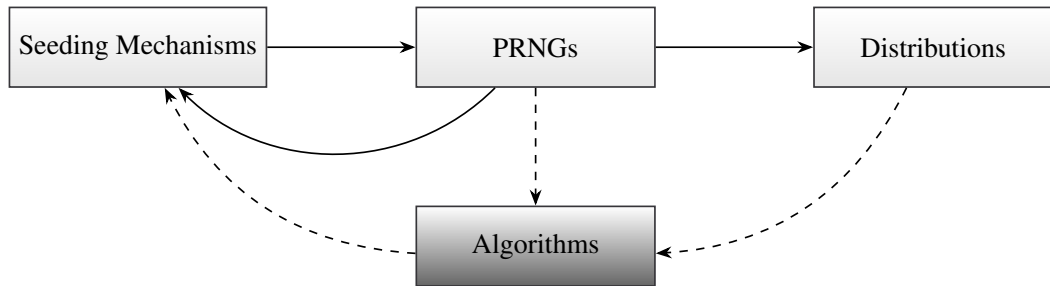
Pseudorandom Number Generator Example



- ▶ construction of “good” PRNG is difficult
- ▶ pseudorandom number sequences will be periodic

Design of the Library

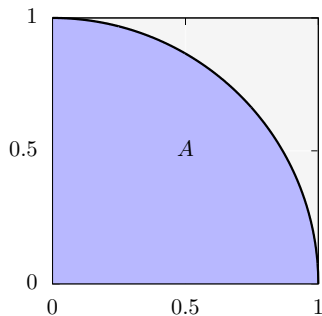
Design Components



Usage in C++

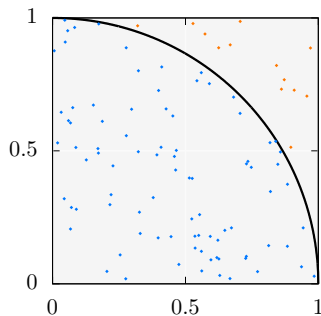
```
#include <pxart/pxart.hpp>
//
std::random_device rd{};
//
pxart::mt19937 rng1{};
pxart::mt19937 rng1{rd};
pxart::mt19937 rng1{pxart::mt19937::default_seeder{rd()}};
//
pxart::xrsr128p rng2{rng1};
//
const auto x = pxart::uniform<float>(rng1);
//
const auto y = pxart::uniform(rng2, -1.0f, 1.0f);
```

Computation of π



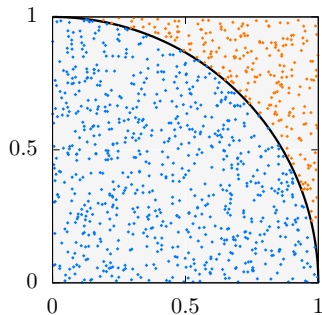
$$A = \frac{\pi}{4}, \quad \hat{\pi} = \frac{4N_A}{N}$$

Computation of π



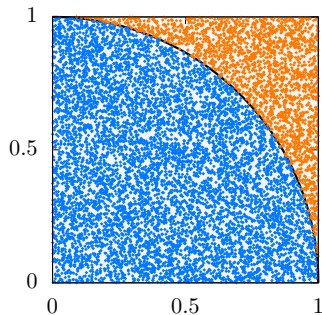
$$A = \frac{\pi}{4}, \quad \hat{\pi} = \frac{4N_A}{N} = \frac{4 \cdot 87}{100} = 3.48$$

Computation of π



$$A = \frac{\pi}{4}, \quad \hat{\pi} = \frac{4N_A}{N} = \frac{4 \cdot 765}{1000} = 3.06$$

Computation of π



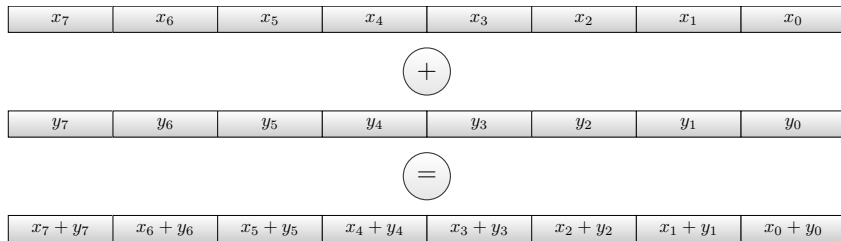
$$A = \frac{\pi}{4}, \quad \hat{\pi} = \frac{4N_A}{N} = \frac{4 \cdot 7856}{10000} = 3.1424$$

Example Usage

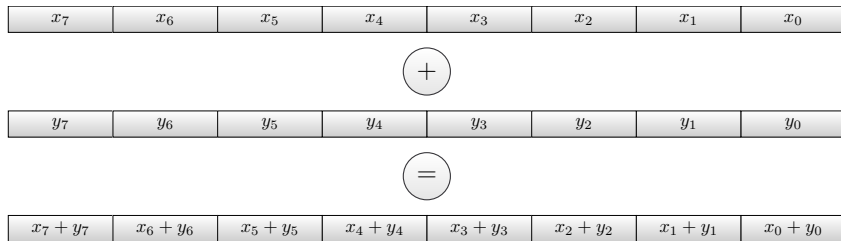
```
// ...  
#include <pxart/pxart.hpp>  
// ...  
pxart::mt19937 rng{};  
const int samples = 100000000;  
int pi = 0;  
for (auto i = samples; i > 0; --i) {  
    const auto x = pxart::uniform<float>(rng);  
    const auto y = pxart::uniform<float>(rng);  
    pi += (x * x + y * y <= 1);  
}  
pi = 4.0f * pi / samples;  
  
// ...
```

Vectorization and SIMD Architectures

SIMD Architecture

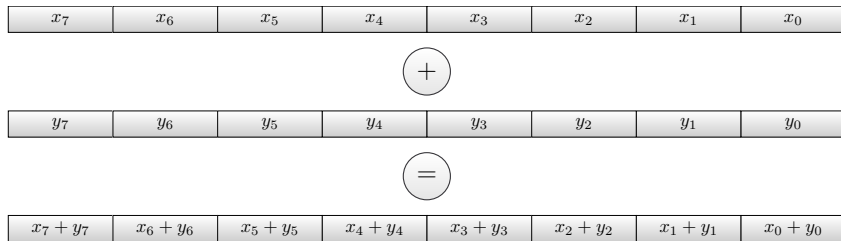


SIMD Architecture



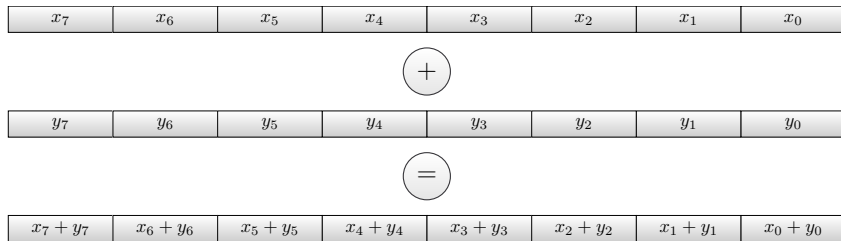
- exploits data-level parallelism on a low level

SIMD Architecture



- ▶ exploits data-level parallelism on a low level
- ▶ Intel CPUs use fixed-length vector registers

SIMD Architecture



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- ▶ Intel CPUs use fixed-length vector registers
- ▶ vector operations are performed on all values at once

SIMD Features in C++

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- ▶ SSE, AVX and AVX512
instruction set features

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- ▶ Assembler Instructions vs. Automatic Vectorization vs. SIMD Intrinsics

SIMD Features in C++

- ▶ SSE, AVX and AVX512 instruction set features
- ▶ Assembler Instructions vs. Automatic Vectorization vs. SIMD Intrinsics

```
// 128-bit registers
```

```
__m128 a;
```

```
__m128d b;
```

```
__m128i c;
```

```
c = _mm_add_ps(a, b);
```

```
// 256-bit registers
```

```
__m256 a;
```

```
__m256i b;
```

```
__m256d c;
```

```
c = _mm256_add_ps(a, b);
```

Why should we vectorize PRNGs manually?

SIMD Architecture

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- ▶ exploit full functionality of today's processors

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- ▶ exploit full functionality of today's processors
- ▶ no automatic vectorization possible
- ▶ other vectorized code needs vectorized random numbers
- ▶ faster generation of numbers
- ▶ PRNGs are low-level, SIMD is low-level

SIMD Architecture

What are conditions for good vectorization?

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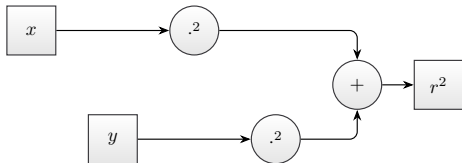
- ▶ nearly no data dependencies
- ▶ same processing pipeline
- ▶ branchless execution
- ▶ CPU-bound algorithms

SIMD Example

$$x, y \in \mathbb{R}, \quad r^2 = x^2 + y^2$$

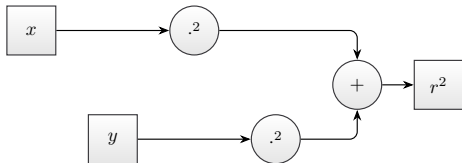
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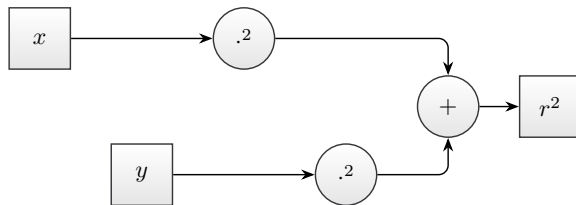
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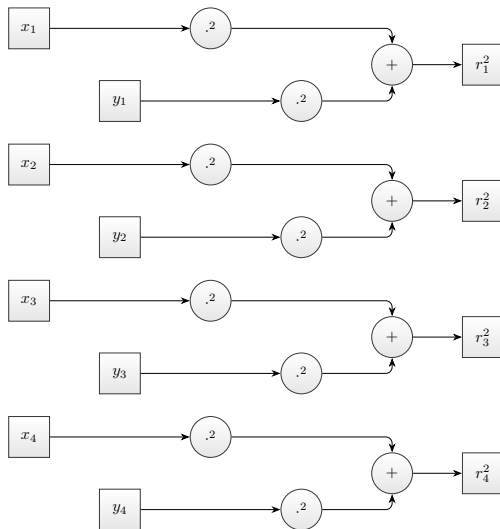
```
double x = pxart::uniform<double>(rng);  
double y = pxart::uniform<double>(rng);
```

```
double x2 = x * x;  
double y2 = y * y;  
double r2 = x2 + y2;
```

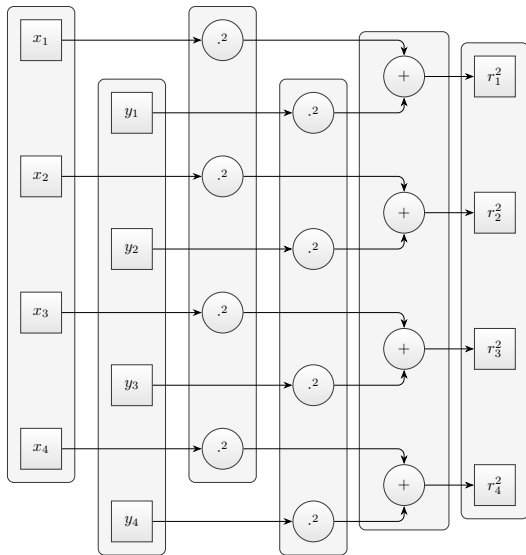

SIMD Example



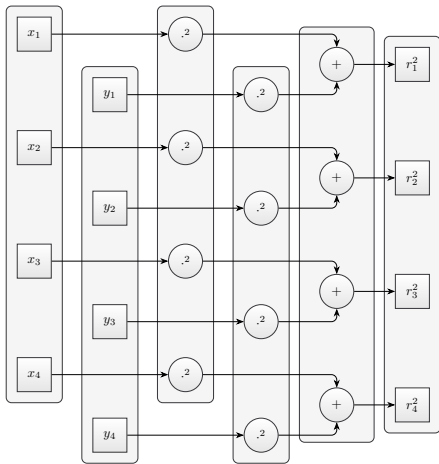
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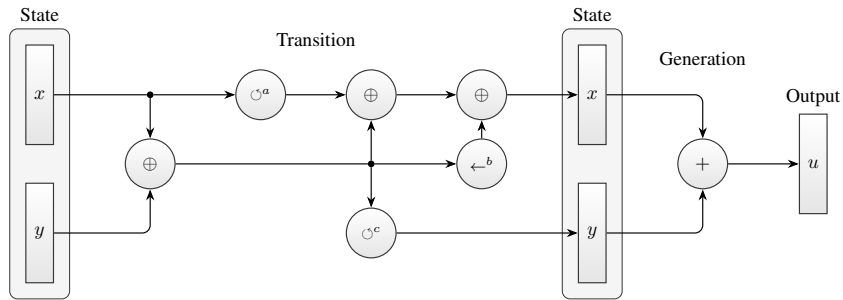
SIMD Example



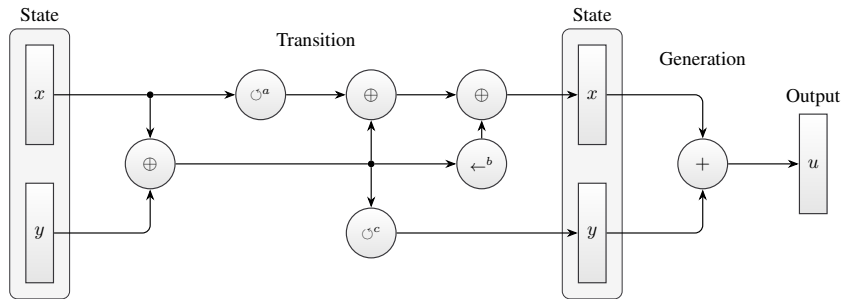
```
__m256d x = pxart::uniform<double>(vrng);  
__m256d y = pxart::uniform<double>(vrng);  
  
__m256d x2 = _mm256_mul_pd(x, x);  
__m256d y2 = _mm256_mul_pd(y, y);  
__m256d r2 = _mm256_add_pd(x2, y2);
```

Implementation of the Xoroshiro128+

Xoroshiro128+ Scheme

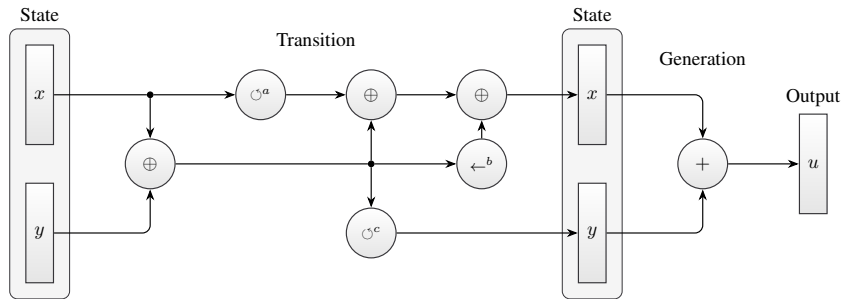


Xoroshiro128+ Scheme



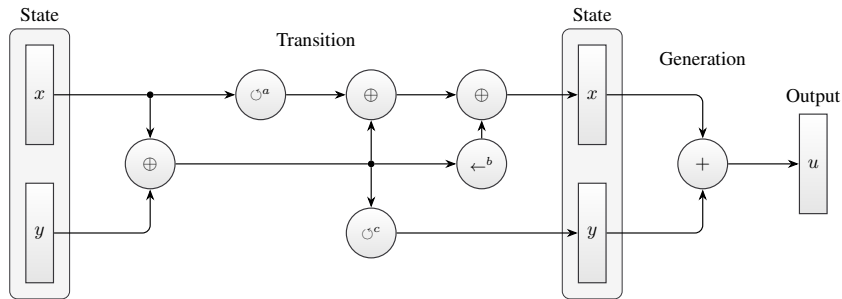
► scrambled linear PRNG

Xoroshiro128+ Scheme



- ▶ scrambled linear PRNG
- ▶ 128-bit state, 64-bit output

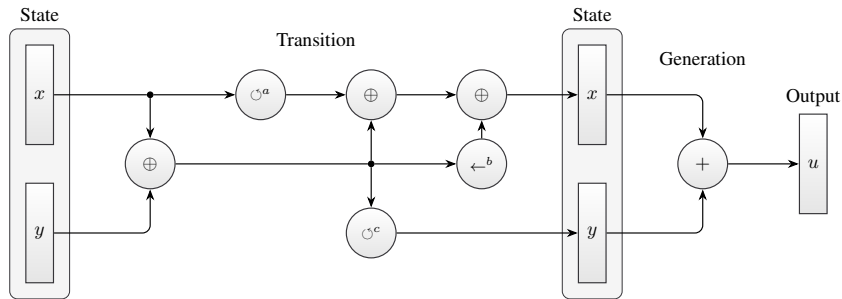
Xoroshiro128+ Scheme



- ▶ scrambled linear PRNG
- ▶ 128-bit state, 64-bit output

▶ period: $2^{128} - 1$

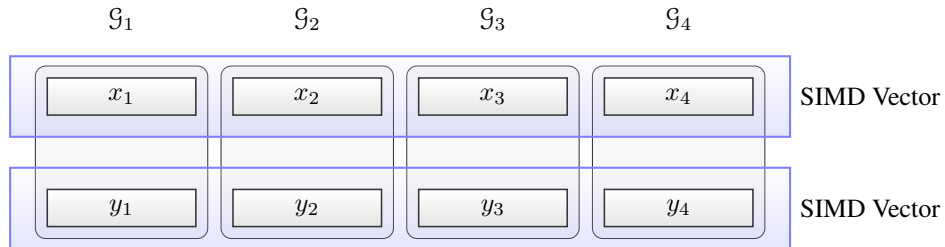
Xoroshiro128+ Scheme



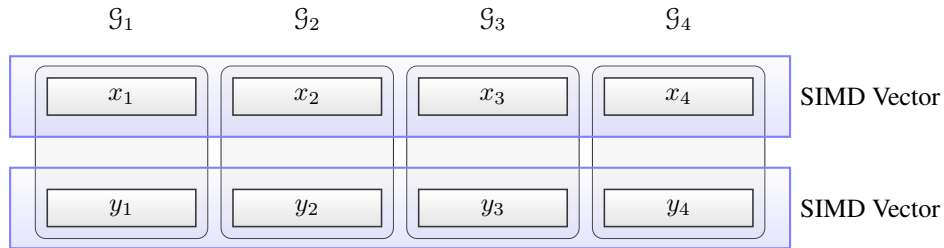
- ▶ scrambled linear PRNG
- ▶ 128-bit state, 64-bit output

- ▶ period: $2^{128} - 1$
- ▶ jump operations

Xoroshiro128+ SIMD Scheme

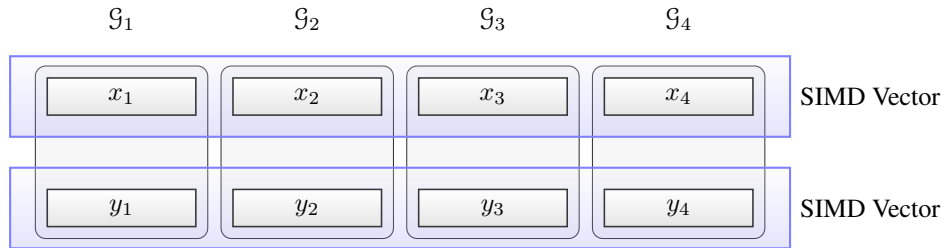


Xoroshiro128+ SIMD Scheme



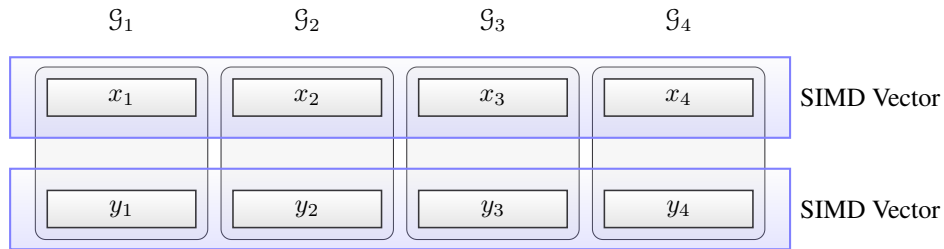
- several parallelization techniques for multiple streams

Xoroshiro128+ SIMD Scheme



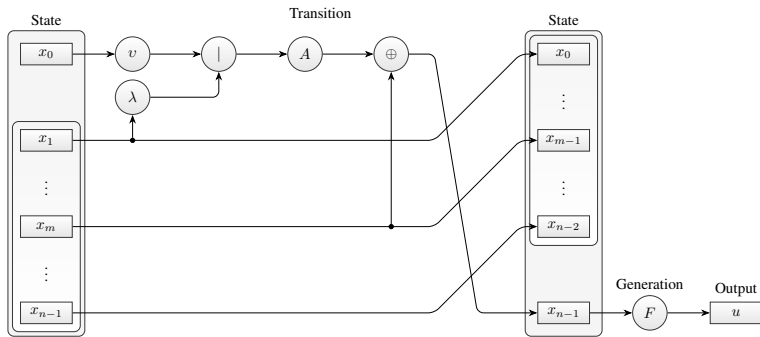
- ▶ several parallelization techniques for multiple streams
- ▶ here: multiple instances of the same generator

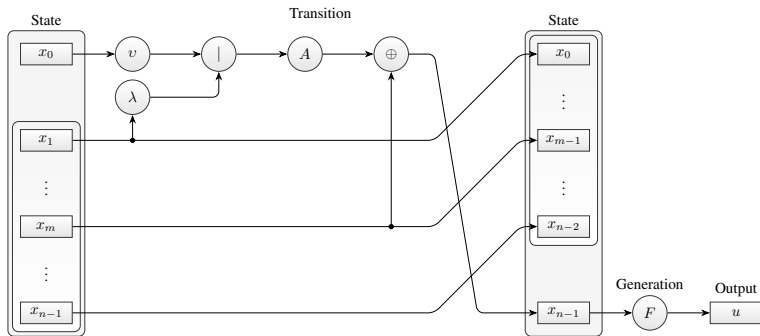
Xoroshiro128+ SIMD Scheme



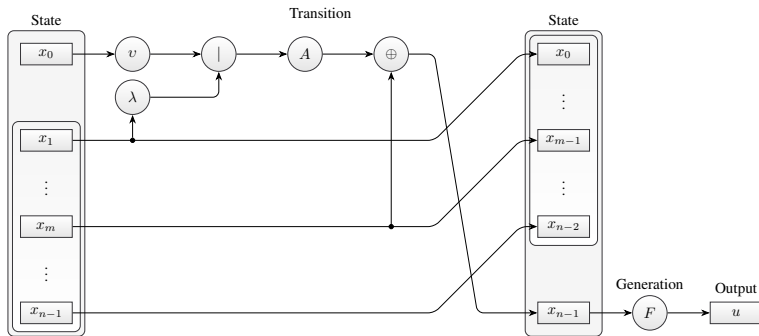
- ▶ several parallelization techniques for multiple streams
- ▶ here: multiple instances of the same generator
- ▶ seeding and parameter variations for multiple streams

Implementation of the MT19937

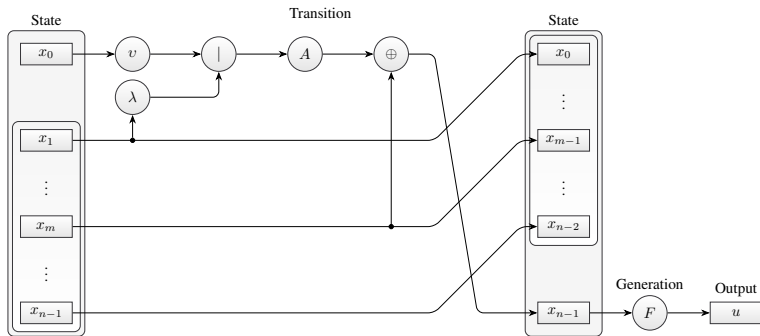




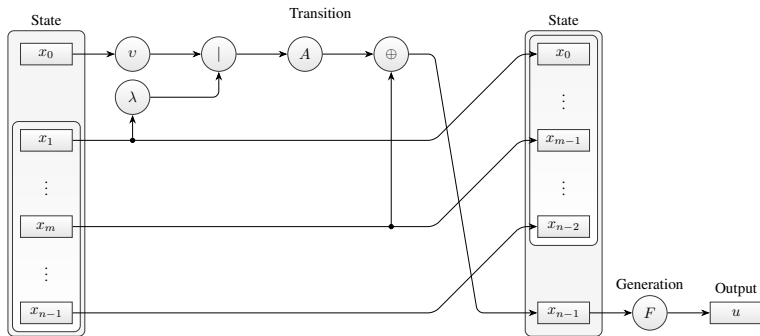
► de-facto standard



- ▶ de-facto standard
- ▶ linear PRNG

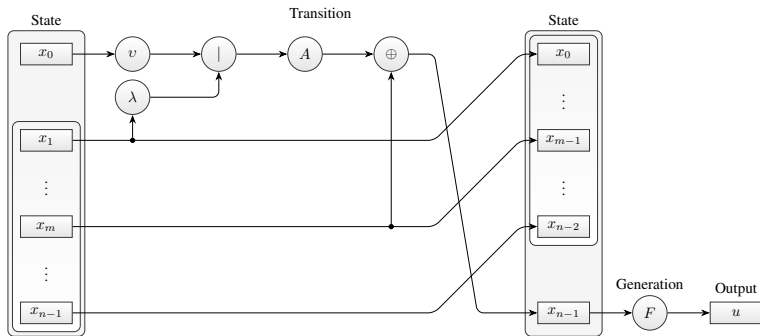


- ▶ de-facto standard
- ▶ linear PRNG
- ▶ 19937-bit state, 32-bit output



- ▶ de-facto standard
- ▶ linear PRNG
- ▶ 19937-bit state, 32-bit output

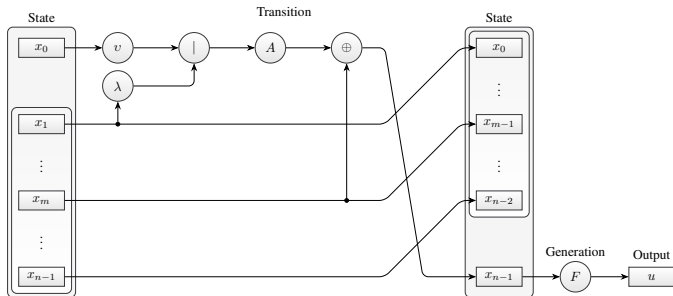
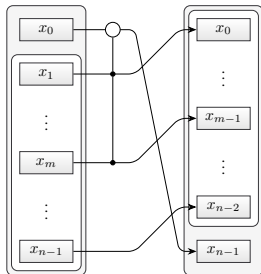
- ▶ period: $2^{19937} - 1$



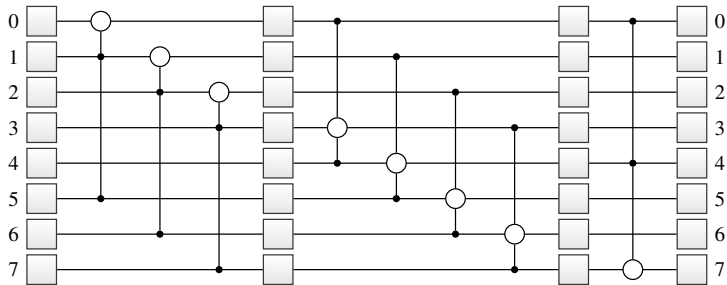
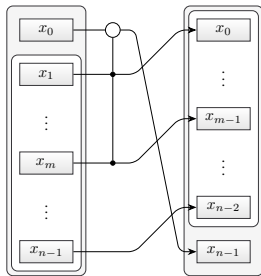
- ▶ de-facto standard
- ▶ linear PRNG
- ▶ 19937-bit state, 32-bit output

- ▶ period: $2^{19937} - 1$
- ▶ 623-dimensional equidistributed

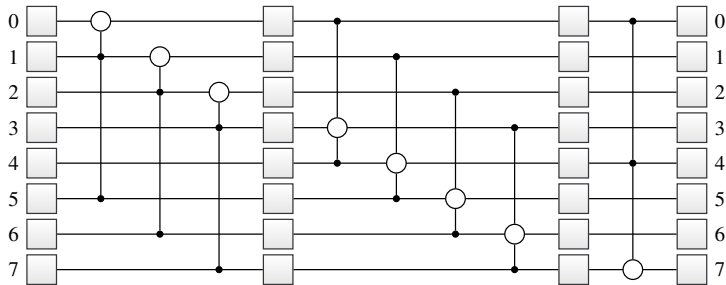
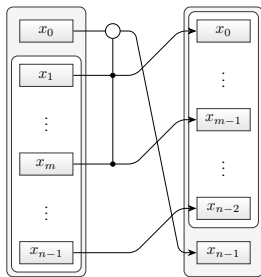
MT19937 Abbreviation



MT19937 Scalar Loop Scheme

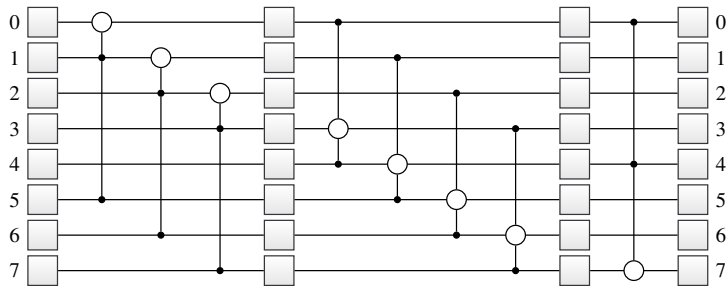
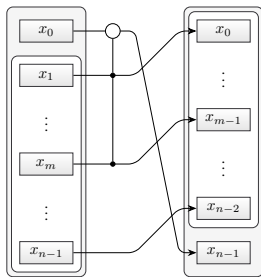


MT19937 Scalar Loop Scheme



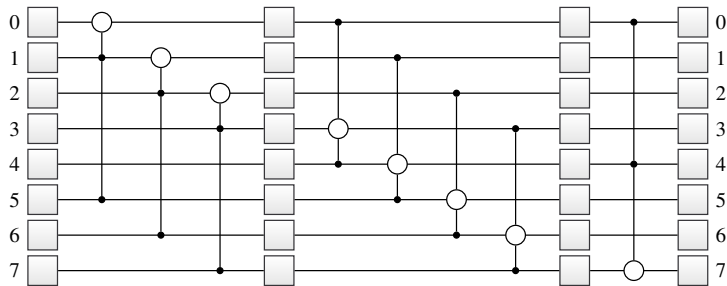
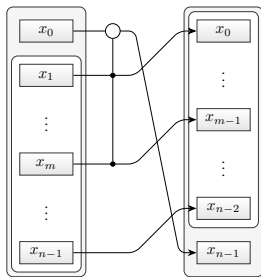
- moving all elements with one transition is inefficient

MT19937 Scalar Loop Scheme



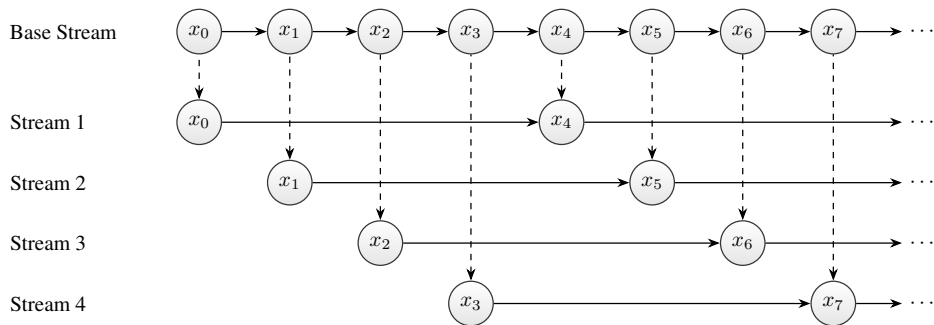
- ▶ moving all elements with one transition is inefficient
- ▶ instead do n transitions at once

MT19937 Scalar Loop Scheme



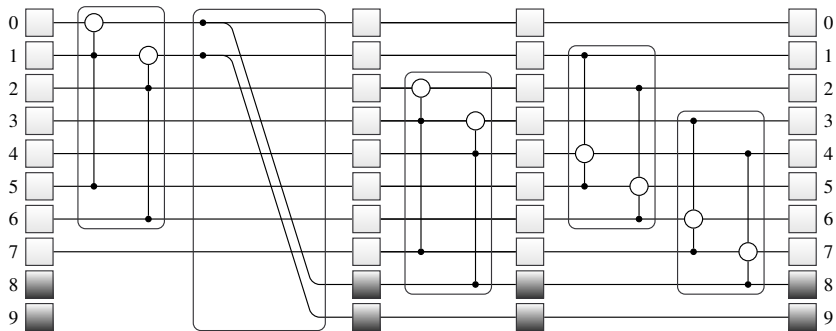
- ▶ moving all elements with one transition is inefficient
- ▶ instead do n transitions at once
- ▶ example with $n = 8$ and $m = 5$; reality with $n = 624$ and $m = 397$

MT19937 SIMD Leap Frogging

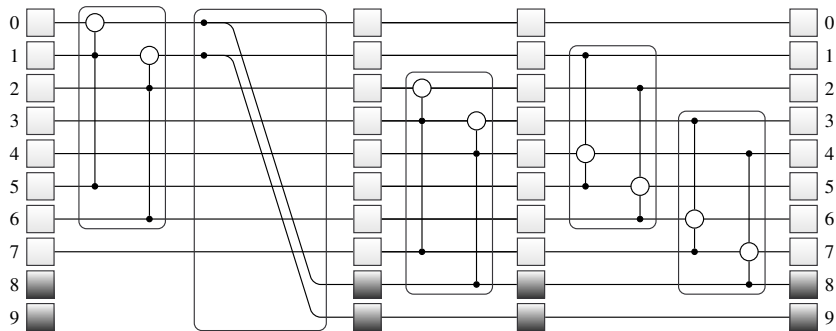


- ▶ vectorized generator will give same output as scalar one, only faster

MT19937 SIMD Loop Scheme

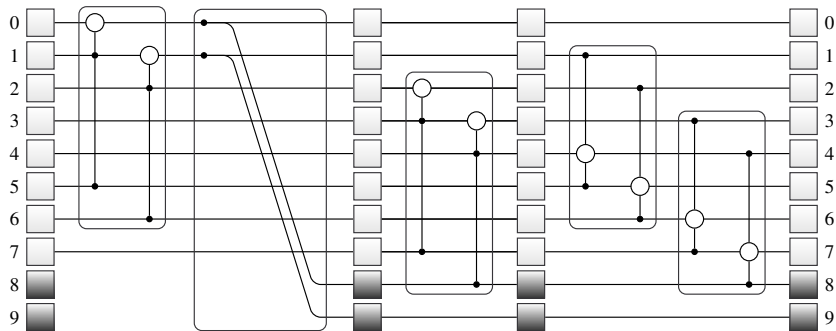


MT19937 SIMD Loop Scheme



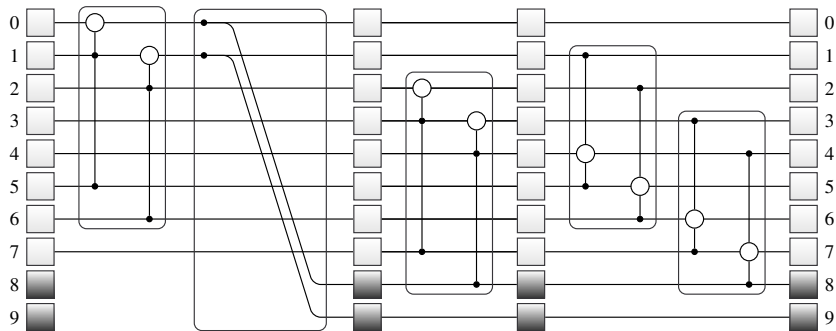
- ▶ example: two-element-vector; reality: up to eight-element-vector

MT19937 SIMD Loop Scheme



- ▶ example: two-element-vector; reality: up to eight-element-vector
- ▶ add vector-register-sized buffer at the end

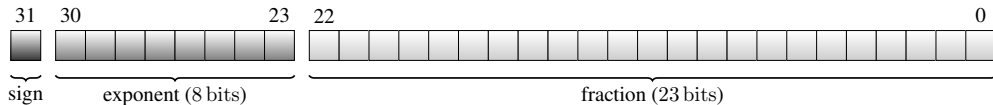
MT19937 SIMD Loop Scheme



- ▶ example: two-element-vector; reality: up to eight-element-vector
- ▶ add vector-register-sized buffer at the end
- ▶ copy generated head to the end and do the vectorized loop

Implementation of Uniform Distribution Functions

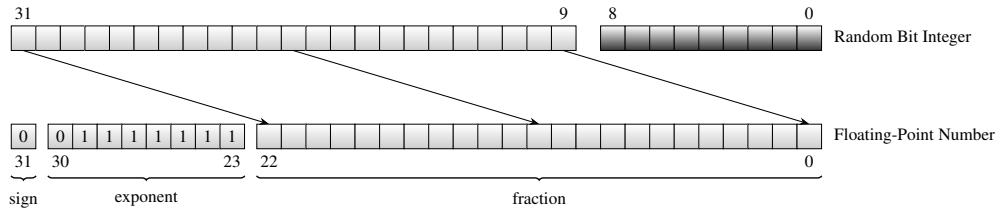
Real Uniform Distribution: Floating-Point Encoding



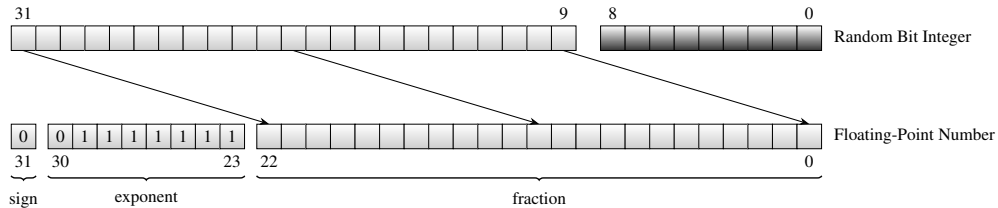
$$x = (-1)^s \cdot m \cdot 2^{e-o}$$

- ▶ IEEE 754
- ▶ we use only normalized numbers

Real Uniform Distribution

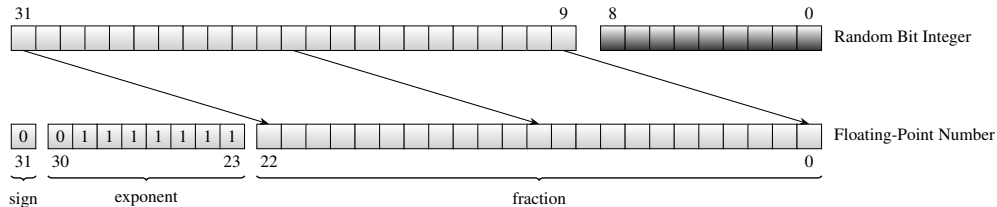


Real Uniform Distribution



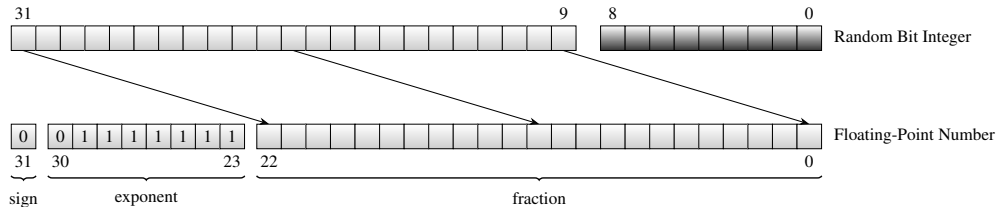
► get random integer

Real Uniform Distribution



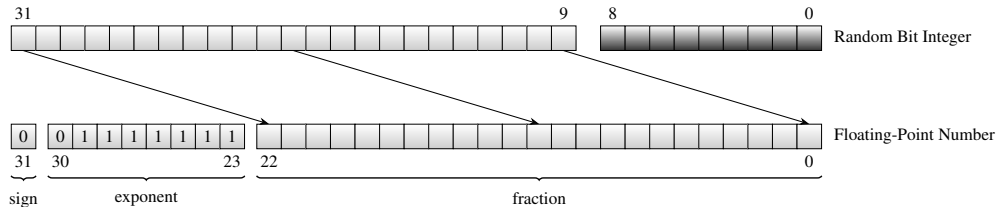
- ▶ get random integer
- ▶ shift bits with highest entropy into fraction part

Real Uniform Distribution



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Real Uniform Distribution



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- ▶ subtract one from result

Integer Uniform Distribution

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- ▶ bias can be neglected for typical simulations

Evaluation and Results

Tests and Performance

Tests and Performance

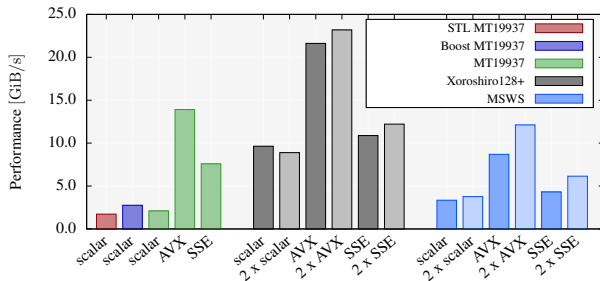
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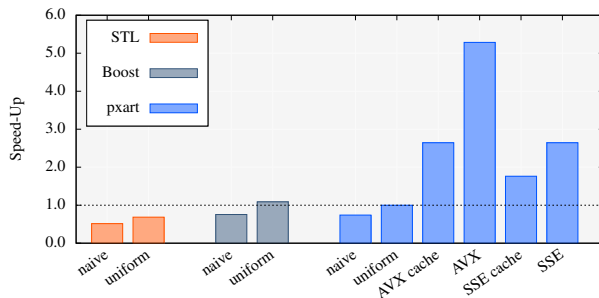
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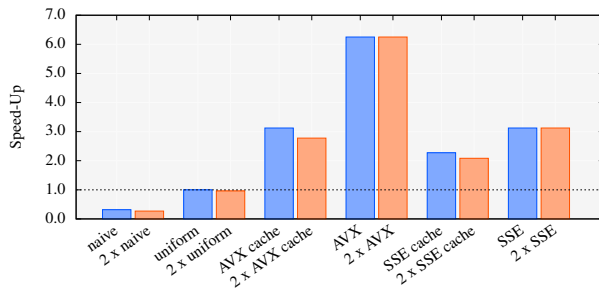
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- Performance: Filling a Cache, Monte Carlo π



MT19937 Speed-Up Monte Carlo π



Xoroshiro128+ Speed-Up Monte Carlo π



Comparison to Intel MKL VSL and RNGAVXLIB

RNGAVXLIB	Intel MKL VSL	Cached AVX	Pure AVX
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- ▶ Intel MKL VSL always fills vector of data
- ▶ benchmarks are biased

Conclusions and Future Work

Comparison

	pXart	RNGAVXLIB	Intel MKL
Portable	✓	✗	✗
User-Friendly API	✓	✗	✗
Header-Only	✓	✗	✗
Open Source	✓	✓	✗
Documentation	✓	✗	~
Distributions	✗	✓	✓
CMake and build2 Support	✓	✗	✗
Dependency-Free	✓	✓	~
Easy-to-get	✓	~	~
AVX512	✗	~	✓

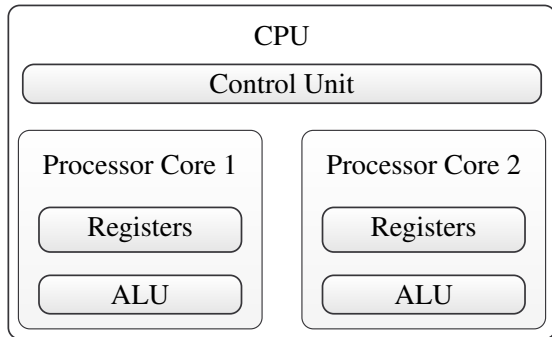
Conclusions and Future Work

- ▶ possible applications in simulations
- ▶ mt19937 vs. xoroshiro128+

Thank you for Your Attention!

References

Processor



Memory Hierarchy

