Simulating spin models on GPU
Lecture 3: Random number generators

Martin Weigel

Applied Mathematics Research Centre, Coventry University, Coventry, United Kingdom and
Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

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Emmy Noether-Programm
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Junior Research Group
"Complex Systems with Frustration"

JG|U

Coventry University

Outline

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  - further distributions (such as Gaussian) generated from transformations
- generally two types of pseudo RNGs considered
  - for general purposes, including simulations
  - or for cryptographic purposes, requiring sufficient randomness to prevent efficient stochastic inference

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VOLUME 69, NUMBER 23 PHYSICAL REVIEW LETTERS 7 DECEMBER 1992

Monte Carlo Simulations: Hidden Errors from "Good" Random Number Generators

Alan M. Ferrenberg and D. P. Landau
Center for Simulational Physics, The University of Georgia, Athens, Georgia 30602

Y. Joanna Wong
IBM Corporation, Supercomputing Systems, Kingston, New York 12401
(Received 29 July 1992)

The Wolff algorithm is now accepted as the best cluster-flipping Monte Carlo algorithm for beating "critical slowing down." We show how this method can yield *incorrect* answers due to subtle correlations in "high quality" random number generators.

PACS numbers: 75.40.Mg, 05.70.Jk, 64.60.Fr

The explosive growth in the use of Monte Carlo simulations in diverse areas of physics has prompted extensive investigation of new methods and of the reliability of both old and new techniques. Monte Carlo simulations are ing model, to study the time correlations, but so far there has been no careful study of the accuracy of the thermodynamic properties which are extracted from the configurations generated by this process.

The story of R250

The New York Times

Technology

Coin-Tossing Computers Found to Show Subtle Bias

By MALCOLM W. BROWNE
Published: January 12, 1993

WHEN scientists use computers to try to predict complex trends and events, they often apply a type of calculation that requires long series of random numbers. But instructing a computer to produce acceptably random strings of digits is proving maddeningly difficult.

In deciding which team kicks off a football game, the toss of a real coin is random enough to satisfy all concerned. But the cost of even a slightly nonrandom string of electronic coin tosses can be devastating to both practical problem-solving and pure theory, and a new investigation has revealed that nonrandom computer tosses are much more common than many scientists had assumed.

Mathematical "models" designed to predict stock prices, atmospheric warming, airplane skin friction, chemical reactions, epidemics, population growth, the outcome of battles, the locations of oil deposits and hundreds of other complex matters increasingly depend on a statistical technique called Monte Carlo Simulation, which in turn depends on reliable and inexhaustible sources of random numbers.

Monte Carlo Simulation, named for Monaco's famous gambling casino, can help to represent very complex interactions in physics, chemistry, engineering, economics and environmental dynamics mathematically. Mathematicians call such a representation a "model," and if a model is accurate enough, it produces the same responses to manipulations that the real thing would do. But Monte Carlo modeling contains a dangerous flaw: if the supposedly random numbers that must be pumped into a simulation actually form some subtle, nonrandom pattern, the entire simulation (and its predictions) may be wrong.

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  - correlation tests
  - comparison to combinatorial identities
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Test batteries:

- DieHard (1995) by G. Marsaglia, now outdated
- TestU01 (2002/2009) by P. L'Ecuyer and co-workers, quasi standard

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  - (c) setup of independent generators of the same class of RNGs using different lags, multipliers, shifts etc.

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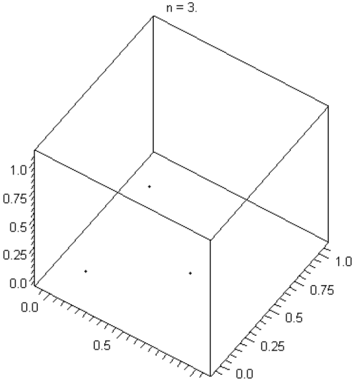

(Source: Wikipedia)

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- can be improved by choosing $m = 2^{64}$ and truncation to 32 most significant bits, period $p = m \approx 10^{18}$ and 8 bytes per thread

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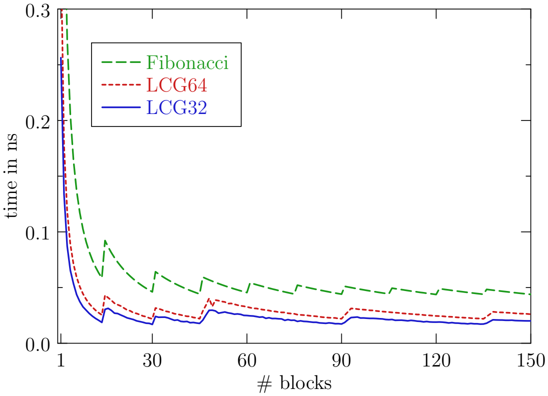
LCG implementation

```
#define MULT32 2.328306437080797e-10f

#define CONVERT(x) (MULT32*((unsigned int)(x)))
//#define CONVERT(x) _curand_uniform(x)
//#define CONVERT(x) __fdividef(__uint2float_rz(x),(float)0x100000000);
```

LCG: performance

How well do they perform?



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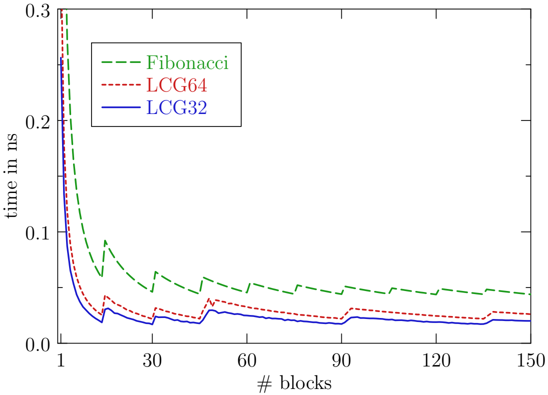

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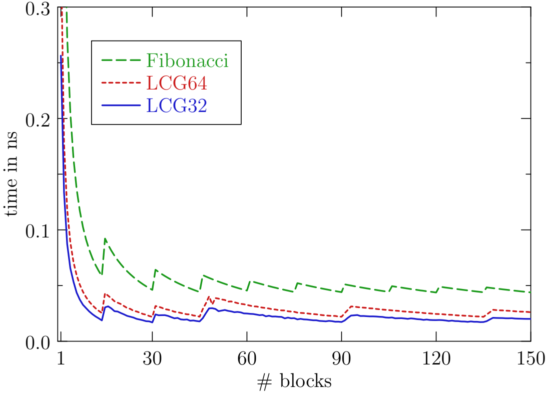

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Peak performance at 58×10^9 (LCG32) and 46×10^9 (LCG64) random numbers per second, respectively.

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Use these LCG generators for the previously developed simulation code for the 2D Ising model. Exact results are available for comparison. Test case of 1024×1024 system at $\beta = 0.4$, 10^7 sweeps.

- checkerboard update uses random numbers in different way than sequential update
- linear congruential generators can skip ahead: "right" way uses non-overlapping sub-sequences
- "wrong" way uses sequences from random initial seeds, many of which must overlap

RNG quality: Ising results

Table: Internal energy e per spin and specific heat C_V for a 1024×1024 Ising model with periodic boundary conditions at $\beta = 0.4$.

method	e	Δ_{rel}	C_V	Δ_{rel}	$t_{\mathrm{up}}^{k=1}$	$t_{\mathrm{up}}^{k=100}$
exact	1.106079207	0	0.8616983594	0		
sequential update (CPU)						
LCG32	1.1060788(15)	−0.26	0.83286(45)	−63.45		
LCG64	1.1060801(17)	0.49	0.86102(60)	−1.14		
Fibonacci, $r = 512$	1.1060789(17)	−0.18	0.86132(59)	−0.64		
checkerboard update (GPU)						
LCG32	1.0944121(14)	−8259.05	0.80316(48)	−121.05	0.2221	0.0402
LCG32, random	1.1060775(18)	−0.97	0.86175(56)	0.09	0.2221	0.0402
LCG64	1.1061058(19)	13.72	0.86179(67)	0.14	0.2311	0.0471
LCG64, random	1.1060803(18)	0.62	0.86215(63)	0.71	0.2311	0.0471
MWC, same a	1.1060800(18)	0.45	0.86161(60)	−0.15	0.2293	0.0435
MWC, different a	1.1060797(18)	0.28	0.86168(62)	−0.03	0.2336	0.0438
Fibonacci, $r = 521$	1.1060890(15)	6.43	0.86099(66)	−1.09	0.2601	0.0661
Fibonacci, $r = 1279$	1.1060800(19)	0.40	0.86084(53)	−1.64	0.2904	0.0700
XORWOW (cuRAND)	1.1060654(15)	−9.13	0.86167(65)	0.04	0.7956	0.0576
XORShift/Weyl	1.1060788(18)	−0.23	0.86184(53)	0.27	0.2613	0.0721
Philox4x32_7	1.1060778(18)	−0.79	0.86109(65)	−0.93	0.2399	0.0523
Philox4x32_10	1.1060777(17)	−0.85	0.86188(61)	0.30	0.2577	0.0622

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- poor for LCG32
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RNG quality: TestU01 results

Table: The memory footprint is measured in bits per thread. For the TestU01 results, if (too many) failures in SmallCrush are found, Crush and BigCrush are not attempted; likewise with failures in Crush. The performance column shows the peak number of 32-bit uniform floating-point random numbers produced per second on a fully loaded GTX 480 device.

generator	bits/thread	failures in TestU01			Ising test	perf.
		SmallCrush	Crush	BigCrush		$\times 10^9$/s
LCG32	32	12	—	—	failed	58
LCG32, random	32	3	14	—	passed	58
LCG64	64	None	6	—	failed	46
LCG64, random	64	None	2	8	passed	46
MWC	$64+32$	1	29	—	passed	44
Fibonacci, $r = 521$	≥ 80	None	2	—	failed	23
Fibonacci, $r = 1279$	≥ 80	None	(1)	2	passed	23
XORWOW (cuRAND)	192	None	None	1/3	failed	19
MTGP (cuRAND)	≥ 44	None	2	2	—	18
XORShift/Weyl	32	None	None	None	passed	18
Philox4x32_7	(128)	None	None	None	passed	41
Philox4x32_10	(128)	None	None	None	passed	30

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General conclusion: fast, but not good enough

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Multiply-with-carry

An only slightly more complicated recursion suggested by Marsaglia is defined by

$$\begin{aligned} x_{n+1} &= a x_n + c_n \pmod{m}, \\ c_{n+1} &= \lfloor (a x_n + c_n)/m \rfloor. \end{aligned}$$

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- $\Rightarrow$ expensive to generate *many* instances, need 64 + 32 bits of state

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- to achieve the full period, one requires $am - 1$ as well as $(am - 2)/2$ to be prime (such that $am - 1$ is a safe prime)
- $\Rightarrow$ expensive to generate *many* instances, need $64 + 32$ bits of state

LCG implementation

```
unsigned long long int ran;
CONVERT((unsigned int)(ran = (ran&0xffffffffull)*AMWC+ran>>32));
```

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Outline

Mersenne twister

See:

M. Mansen, M. Weigel, and A. K. Hartmann, Eur. Phys. J. Special Topics 210, 53 (2012.)

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```
__device__ state_t rng_update(state_t state, int tid,
                              volatile state_t* stateblock)
{
/* Indices. */
int wid = tid / WARPSIZE; // Warp index in block
int lid = tid % WARPSIZE; // Thread index in warp
int woff = wid * (WARPSIZE + WORDSHIFT + 1) + WORDSHIFT + 1;
                                          // warp offset
/* Shifted indices. */
int lp = lid + WORDSHIFT; // Left word shift
int lm = lid - WORDSHIFT; // Right word shift

/* << A. */
stateblock[woff + lid] = state; // Share states
state ^= stateblock[woff + lp] << RAND_A; // Left part
state ^= stateblock[woff + lp + 1] >> WORD - RAND_A; // Right part

/* >> B. */
stateblock[woff + lid] = state; // Share states
state ^= stateblock[woff + lm - 1] << WORD - RAND_B; // Left part
state ^= stateblock[woff + lm] >> RAND_B; // Right part

/* << C. */
stateblock[woff + lid] = state; // Share states
state ^= stateblock[woff + lp] << RAND_C; // Left part
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return state;
}
```

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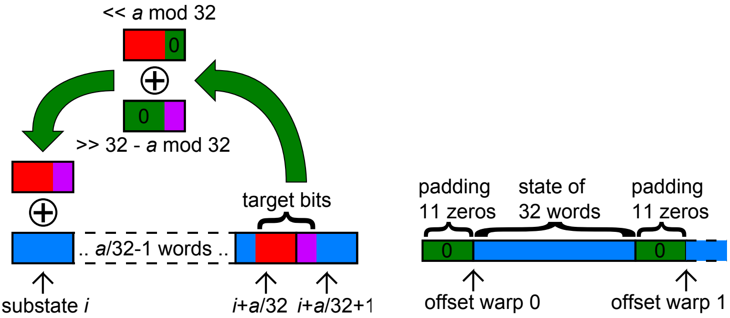

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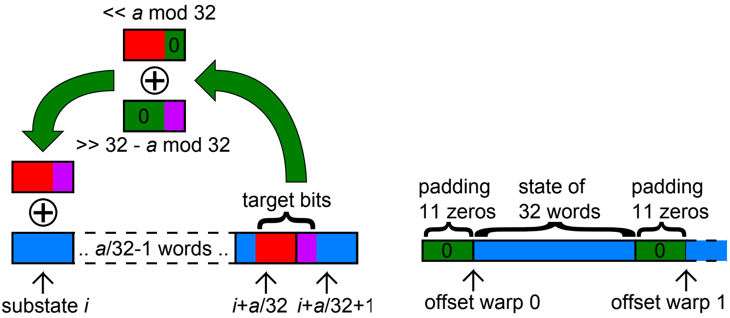

- due to single-thread scheduling, no thread synchronization is required
- use `volatile` keyword to ensure writes
- use skip-ahead to create sub-streams
- combine with Weyl generator, $y_n = (y_{n-1} + c) \mod 2^w$, to further improve quality

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Cryptographic generators

For the Weyl generator above, we can evaluate the n element in one step,

$$y_n = (y_0 + nc) \mod 2^w.$$

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Well-known and proven symmetric-key cryptosystems are DES and AES.

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$$[L_n][R_n \oplus f(L_n, K_n)] = [R_{n-1}]\;[L_{n-1} \oplus f(R_{n-1}, K_n) \oplus f(L_n, K_n)] = [R_{n-1}]\;[L_{n-1}],$$

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where $f(R_{n-1}, K_n) \oplus f(L_n, K_n) = 0$ since $L_n = R_{n-1}$. Continuing with the key sequence K_n, K_{n-1}, ..., K_0, we arrive at R_0L_0 and hence L_0R_0.

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$$e(m_1 m_2 m_3 m_4 m_5 m_6) = m_1 m_2 m_4 m_3 \; m_4 m_3 m_5 m_6,$$

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- We derive the key K_i for round i from $K = k_0 k_1 k_2 k_3 k_4 k_5 k_6 k_7 k_8$ by

$$K_i = k_{(i-1) \mod 9} k_{i \mod 9} k_{(i+1) \mod 9} \cdots k_{(i+6) \mod 9}.$$

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- In a third step, these 8 bits are passed through one of two S-boxes,

  $$S_1 = \begin{bmatrix} 101 & 010 & 001 & 110 & 011 & 100 & 111 & 000 \\ 001 & 100 & 110 & 010 & 000 & 111 & 101 & 011 \end{bmatrix}$$

  $$S_2 = \begin{bmatrix} 100 & 000 & 110 & 101 & 111 & 001 & 011 & 010 \\ 101 & 011 & 000 & 111 & 110 & 010 & 001 & 100 \end{bmatrix}$$

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For the S-boxes, the 8 bits from step two are broken into two 4-bit parts. The first part is sent to S_1 and the second part to S_2. The first bit of each part selects the row in the S-box, the remaining three bits the column.

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$$e(100110) \oplus K_i = 10101010 \oplus 01100101 = 1100\,1111.$$

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A successful approach to cryptosystems of the DES type is differential cryptanalysis (which was suggested by Biham and Shamir in 1990 but was, in fact, known to the inventor of DES in 1979):

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Philox et al.

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$$\begin{aligned} L' &= \mathrm{mullo}(R, M), \\ R' &= \mathrm{mulhi}(R, M) \oplus k \oplus L, \end{aligned}$$

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Philox-Nxw_r

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- this ensures identical results independent of the parallel setup

RNG quality: Ising results

Table: Internal energy e per spin and specific heat C_V for a 1024×1024 Ising model with periodic boundary conditions at $\beta = 0.4$.

method	e	Δ_{rel}	C_V	Δ_{rel}	$t_{\mathrm{up}}^{k=1}$	$t_{\mathrm{up}}^{k=100}$
exact	1.106079207	0	0.8616983594	0		
sequential update (CPU)						
LCG32	1.1060788(15)	−0.26	0.83286(45)	−63.45		
LCG64	1.1060801(17)	0.49	0.86102(60)	−1.14		
Fibonacci, $r = 512$	1.1060789(17)	−0.18	0.86132(59)	−0.64		
checkerboard update (GPU)						
LCG32	1.0944121(14)	−8259.05	0.80316(48)	−121.05	0.2221	0.0402
LCG32, random	1.1060775(18)	−0.97	0.86175(56)	0.09	0.2221	0.0402
LCG64	1.1061058(19)	13.72	0.86179(67)	0.14	0.2311	0.0471
LCG64, random	1.1060803(18)	0.62	0.86215(63)	0.71	0.2311	0.0471
MWC, same a	1.1060800(18)	0.45	0.86161(60)	−0.15	0.2293	0.0435
MWC, different a	1.1060797(18)	0.28	0.86168(62)	−0.03	0.2336	0.0438
Fibonacci, $r = 521$	1.1060890(15)	6.43	0.86099(66)	−1.09	0.2601	0.0661
Fibonacci, $r = 1279$	1.1060800(19)	0.40	0.86084(53)	−1.64	0.2904	0.0700
XORWOW (cuRAND)	1.1060654(15)	−9.13	0.86167(65)	0.04	0.7956	0.0576
XORShift/Weyl	1.1060788(18)	−0.23	0.86184(53)	0.27	0.2613	0.0721
Philox4x32_7	1.1060778(18)	−0.79	0.86109(65)	−0.93	0.2399	0.0523
Philox4x32_10	1.1060777(17)	−0.85	0.86188(61)	0.30	0.2577	0.0622

RNG quality: TestU01 results

Table: The memory footprint is measured in bits per thread. For the TestU01 results, if (too many) failures in SmallCrush are found, Crush and BigCrush are not attempted; likewise with failures in Crush. The performance column shows the peak number of 32-bit uniform floating-point random numbers produced per second on a fully loaded GTX 480 device.

generator	bits/thread	failures in TestU01			Ising test	perf.
		SmallCrush	Crush	BigCrush		$\times 10^9$/s
LCG32	32	12	—	—	failed	58
LCG32, random	32	3	14	—	passed	58
LCG64	64	None	6	—	failed	46
LCG64, random	64	None	2	8	passed	46
MWC	$64 + 32$	1	29	—	passed	44
Fibonacci, $r = 521$	≥ 80	None	2	—	failed	23
Fibonacci, $r = 1279$	≥ 80	None	(1)	2	passed	23
XORWOW (cuRAND)	192	None	None	1/3	failed	19
MTGP (cuRAND)	≥ 44	None	2	2	—	18
XORShift/Weyl	32	None	None	None	passed	18
Philox4x32_7	(128)	None	None	None	passed	41
Philox4x32_10	(128)	None	None	None	passed	30

Summary and outlook

This lecture

This lecture has given a survey of random number generators in a massively parallel environment. On GPUs, we need a massive number of independent RNGs with small state. Two strategies have been explored: individual generators with small states which, however, suffer from small periods and state-sharing among several instances. An independent alternative are counter-based generators.

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Reading

- M. Manssen, M. Weigel, and A. K. Hartmann, Eur. Phys. J. Special Topics **210**, 53 (2012) [arXiv:1204.6193].