Random number generators for massively parallel simulations on GPU

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Abstract. High-performance streams of (pseudo) random numbers are crucial for the efficient implementation for countless stochastic algorithms, most importantly, Monte Carlo simulations and molecular dynamics simulations with stochastic thermostats. A number of implementations of random number generators has been discussed for GPU platforms before and some generators are even included in the CUDA supporting libraries. Nevertheless, not all of these generators are well suited for highly parallel applications where each thread requires its own generator instance. For this specific situation encountered, for instance, in simulations of lattice models, most of the high-quality generators with large states such as Mersenne twister cannot be used efficiently without substantial changes. We provide a broad review of existing CUDA variants of random-number generators and present the CUDA implementation of a new massively parallel high-quality, high-performance generator with a small memory load overhead.

1 Introduction

In the field of computer simulations [1], the construction of suitably good and fast pseudo-random number generators (RNGs) has been a long-standing problem [2]. This is mostly due to it being ill defined since, as John von Neumann put it, "anyone who considers arithmetical methods of producing random digits is, of course, in a state of sin" [3]. In other words, true random numbers cannot be produced from purely deterministic algorithms and hence the degree to which the thus generated sequences of numbers resemble random sequences is relative. A number of notoriously bad RNGs had been implemented as part of standard libraries on the computer systems available in the early days of computer simulations see, e.g., Ref. [4]. To separate the wheat from the chaff, a number of collections or "batteries" of tests, comparing statistical properties of pseudo-random sequences to those expected for a true random process, have been suggested and extensively used in the past. While for many years Marsaglia's DIEHARD suite [5] was considered the gold standard in the field, with the increase in computer power and the ensuing higher statistical precision of simulations more stringent criteria have to be applied and so to today's standards

one would tend to require a generator to pass the SmallCrush, Crush and BigCrush test series suggested by L'Ecuyer and coworkers in the framework of the TestU01 suite [6].

Since, by definition, a pseudo RNG sequence is the result of a deterministic algorithm, for each generator one can, in principle, construct tests that show that the resulting sequences are not truly random. While the mentioned test batteries check for general statistical flaws of the produced numbers, passing all tests does not guarantee that a given generator does not lead to systematic deviations when used in a Monte Carlo simulation of a specific system. In fact, such application tests serve as additional checks and have repeatedly helped to expose flaws in generators [7,8]. Of particular value for such testing are non-trivial models where exact solutions are available to allow for detecting significant deviations without the need for simulations using other generators. A most useful example in this respect is the two-dimensional Ising ferromagnet, for which exact expressions for finite systems can be easily computed [9].

With the increasing interest in harvesting the superior parallel performance of graphics processing units (GPUs) for general computational purposes [10], these devices have also been discovered by researchers using Monte Carlo and molecular dynamics simulations as convenient means of pushing the limits in studies of notoriously difficult problems. Within a rather wide range of applications, lattice spin systems with short-range interactions appear to benefit particularly well from the massive parallelism of these devices [11-15]. In these systems, the large-scale parallelism of threads and blocks is typically translated into parallel updates of spins on non-interacting sub-lattices. A similar situation, only with possibly a larger number of arithmetic operations interspersed with the consumption of random numbers, is encountered for simulations of molecular and other off-lattice systems [16, 17]. To allow for efficient scaling to the large numbers of threads required for the more and more powerful GPU devices available, the central generation and distribution of random numbers by dedicated CPU or GPU threads is not an option. Instead, each updating unit requires a distinct instance of a RNG. Moreover, many calculations on GPU are rather limited by the bandwidth than by the number and speed of available arithmetic units [18]. To ensure good performance, RNG related accesses to the device global memory must hence be kept at a minimum. As a consequence, random number generators for such massively parallel GPU simulations must fulfill requirements rather different from those for the traditional, serial, CPU based simulations: (a) it must be possible to set up a large number (thousands up to millions) of RNGs that deliver sufficiently uncorrelated streams of random numbers and (b) to minimize memory transfers, the generator states should be stored in local, shared memory, which is very limited.

The problem of parallel generation of random numbers is not completely new (see, e.g., Ref. [19]), but with the number of threads, say, in a multiple-GPU simulation counting in the millions, it is brought to a new level. Different strategies are conceivable here: (1) division of the stream of a long-period generator into non-overlapping sub-streams to be produced and consumed by the different threads of the application, (2) use of very large period generators such that overlaps between the sequences of the different instances are improbable, if each instance is seeded differently, or (3) setup of independent generators of the same class of RNGs using different lags, multipliers, shifts etc. Note that even if a given generator produces pseudo-random sequences of good quality (according to the standard tests), a division into sub-sequences and the ensuing different order in which the numbers are consumed, can lead to much stronger correlations and, hence, worse quality than for the original generator (see the discussion in Sec. 2 below). A rather elegant solution to the problem of indepen-

dent generators was recently suggested in Ref. [20] and will be discussed below in Sec. 7.

The need to minimize memory transfers and hence ensure that the generator states can be stored in shared memory seems to ask for RNGs with very small states. This appears to rule out many of the generators popular for simulations on CPU. The Mersenne twister [21], for instance, has a state of 624 words or about 20 kB which, compared to the 48 kB of shared memory available to up to 1536 threads on an NVIDIA Fermi GPU, is huge. As a rule of thumb, however, RNGs with a larger state lead to larger periods and, in many cases, better statistical quality. To solve this dilemma, two different strategies spring to mind: (1) the search for generators with very small state, but good quality or (2) an attempt to share the state between the threads of a single block and let these threads cooperate to generate many random numbers from the same state in a vectorized call. As we will see below, attempts to use the first approach with conventional generators generally do not lead to satisfactory results. Notably, however, the concept of counter-based, stateless generators of Ref. [20] discussed below seems to be an interesting exception. The concept of state sharing is found, in general, to be more successful. In Sec. 6 below, we discuss a new and efficient generator designed along these lines, that passes all statistical tests. Another difference between the CPU and GPU environments concerns the number of random numbers produced and consumed on each invocation. While it is customary for many optimized CPU RNGs to produce and store a significant number of entries in one (possibly vectorized) call and store the produced numbers for later consumption, this is not feasible for GPU generators with many threads consuming numbers in parallel and in the presence of the memory limitations mentioned above.

Although research into RNGs suitable for GPUs is still at its beginning, a number of such implementations has been discussed previously [11,13,16,20,22–29]. To meet the design goal of a small memory footprint, we deliberately restrict our discussion to generators using up to four machine words (128 bits) of state information per thread. This appears to be about the upper limit for reaching good performance on the present hardware for the massively parallel applications discussed here. This rules out a number of implementations of general-purpose generators [23], such as XORWOW, a multiple recursive XORShift generator proposed by Marsaglia [30], implemented in the cuRAND library [22] (which has 192 bits of state) as well as the standard Mersenne twister implementation in the CUDA SDK (now superseded by MTGP [26]). We shortly discuss these generators for completeness, however. For lack of space, we also here concentrate on CUDA implementations and do not discuss RNGs on ATI cards which have slightly different limitations [27]. Unless stated otherwise, all test runs and benchmarks have been performed with the CUDA 4.0 Toolkit. Finally, we do not here consider the generation of quasi-random numbers. In Sects. 2 and 3 below, we focus on simple generators with small states, whereas in the following Sects. (with the exception of Sec. 7) the state-sharing approach is discussed. All generators are benchmarked in terms of the quality of random numbers by using the Test U01 suite, simulations of the 2D Ising ferromagnet as an application test and GPU performance measurements.

2 Linear-congruential generators

Arguably the simplest and clearly the best understood RNGs [31] are the linear congruential generators of the form

$$x_{n+1} = ax_n + c \pmod{m}. (1)$$

To convert the resulting sequence of integers to (uniformly distributed) numbers in the interval [0,1], one uses the simple output function $u_n=x_n/m$. If appropriate constants a, c, and m are chosen, the period of this class of generators is p=m. Since for efficient implementations it is inconvenient (and usually not computationally efficient) to make m larger than the largest integer representable in a native integer type, one is restricted to $m \leq 2^{64}$ on standard architectures. Hence, the achievable periods are rather small to today's standards. What is more, on theoretical grounds it is argued that one actually should not use more than \sqrt{p} numbers out of such a sequence [2,31]. Indeed, for $m=2^{32}$ a simulation of a 4096×4096 Ising system, for instance, would use p numbers in only 256 sweeps. The choices $m=2^{32}$ or $m=2^{64}$ have the advantage that there is no need to perform the modulo operation explicitly since on most modern architectures (including GPUs) integer overflows are equivalent to taking a modulo operation. For such power of two moduli m, however, the period of the less significant bits is even shorter than that of the more significant bits, such that the period of the kth least significant bit is only 2^k .

An advantage for the parallel calculations performed here is that one can easily skip ahead in the sequence, observing that

$$x_{n+t} = a_t x_n + c_t \pmod{m},\tag{2}$$

where

$$a_t = a^t \pmod{m}, \quad c_t = \sum_{i=1}^t a^i c \pmod{m}.$$
 (3)

Therefore, choosing t equal to the number of threads consuming random numbers, all threads can generate numbers out of the same global sequence (1) concurrently. This corresponds to the sub-streams approach of parallel random number generation mentioned above. An alternative setup, that cannot guarantee the desired independence of the sequences associated to individual RNG instances, however, starts from randomized initial seeds for each generator, without using any skipahead [11]. A potentially safer approach of choosing independent constants a and c for each instance while keeping m unchanged does not appear to be feasible since there are not enough multipliers with good properties available for massively parallel simulations [32]. For our tests with $m = 2^{32}$, we used a = 1664525 and $c = 1013\,904\,223$, originally suggested in Ref. [33]. Moving on to 64-bit, and hence increasing the memory footprint to two machine words, gives a somewhat more reasonable, but still short period $p=2^{64}\approx 2\times 10^{19}$. As multiplier we here chose a = 2862933555777941757 with provably relatively good properties [32], where an odd offset, here c = 1442695040888963407, needs to be chosen to reach the maximal period.

It is well-known that unmodified LCGs have rather bad statistical properties. In particular, plotting k-tuples of successive (normalized) numbers as points in \mathbb{R}^k , even for rather small k the points are found to be confined to a sequence of hyperplanes instead of being uniformly distributed. Applying the tests of the TestU01 suite, we find that our 32-bit generator LCG32 already fails 12 out of the 15 tests of the SmallCrush battery, such that we did not even attempt the Crush and BigCrush tests. The results are summarized in Table 2. In a parallel GPU code, this original order of using the produced numbers corresponds to using skip-ahead according to Eq. (2). The alternative approach of randomly initializing each parallel instance of the generator with a different RNG without any skipping provisions leads to somewhat better results as shown in the line "LCG32, random" in Table 2, such that most SmallCrush tests are passed, but the generator fails 14 out of 144 tests in the Crush suite. The 64-bit LCGs pass SmallCrush without failures, but have some problems

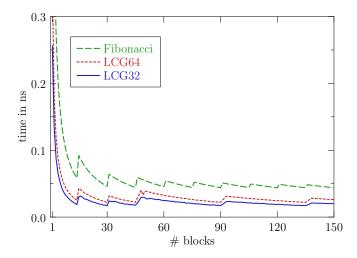


Fig. 1. GPU time per random number for running different implementations of pseudo RNGs on a GTX 480 as a function of the number of grid blocks employed. The Fibonacci generator uses r=521 and s=353. All thread blocks have 512 threads.

in Crush. The randomized variant of LCG64, in particular, tested with a number of 262144 threads (as would be required in a simulation of a 1024×1024 Ising ferromagnet discussed below), fails a moderate 5 out of 196 tests in BigCrush (with an additional 3 suspicious results also counted as failures in Table 2) and could thus almost be considered acceptable.

In addition to the generic tests provided by TestU01, we also performed an application test in the form of a Metropolis simulation of a zero-field, nearest-neighbor Ising ferromagnet on the square lattice. The GPU simulation code employed has been discussed in detail in Refs. [13, 25]. It uses a double checkerboard decomposition which, if mimicked in a serial code, would result in a specific order of using the random numbers. While this is only one particular example problem, its discrete nature makes it relatively likely for flaws in the used RNGs to show up in statistically significant deviations already of basic quantities. While some deviations have been specifically observed for cluster updates [7], which we do not consider here (see, however, Ref. [34]), one could argue that the Ising model is amongst the problems in lattice spin systems that is most sensitive to RNG correlations. In particular, disordered systems that have extra (preferably high-quality) randomness from quenched parameters in the Hamiltonian or continuous-spin models with the resulting continuous probability distributions, are less likely to be afflicted with problems resulting from flawed RNGs. Due to the availability of exact results for the internal energy per site e and specific heat C_V on finite lattices [9], statistical significance of deviations can be easily detected. For the generators discussed here, we used a simulation of a 1024×1024 system with a total of 10^7 sweeps after equilibration to determine e and C_V at the inverse temperature $\beta = 0.4$. As shown in Table 1 the 32-bit LCG, in particular, leads to highly significant deviations in this example. What is more, these deviations are aggravated in the GPU implementation by it sampling from the same random-number sequence via skipping, but using random numbers in a different order. If, on the other hand, the "LCG32, random" variant is used, the deviations go away. As could be expected from the TestU01 results, the deviations produced by the 64-bit flavor are significantly smaller and, again, disappear for the variant with random seeds on GPU.

While the quality of pseudo-randomness is questionable, this class of generators excels, however, in terms of its peak performance on GPU. In Fig. 1, we show the average time for generating a normalized random number uniformly distributed in [0,1] on fully loading a GTX 480 device with generator threads. The characteristic zig-zag pattern results from the number of blocks being more or less commensurate with the number of available multiprocessors on the GPU (which is 15 for the GTX 480used for these tests). The peak performance for the LCG32 is around 58×10^9 random numbers per second, whereas LCG64 yields 46×10^9 numbers per second. Note that for the latter generator, we only use the 32 most significant bits and hence generate only one random number per 64-bit calculation; on using the whole state to produce two 32-bit numbers, the nominal performance would double (but, of course, the quality of the generated numbers would be reduced). These performance measures depend on how many numbers are produced with one generator before the next generator state needs to be loaded from global memory. Hence, while the performance numbers given in Table 2 are from compute-bound calculations and thus reflect the complexity of the arithmetic calculations to produce a new random number, in many practical applications only a few numbers are produced before the state of a generator needs to be written back to global memory, such that in these memory-bound cases run-times are rather dominated by the number of fetches from global memory required to load the generator state. This second type of performance measure is reflected in the speed of the Ising simulation as shown in Table 1. Here, the results for updating the spins of a tile once (k = 1) correspond to the situation that only two random numbers are produced per state load and save operation, whereas for the simulation with multi-hit updates (k = 100), 200 random numbers are produced per access to global memory. The good performance and ease of implementation are plausible reasons for this type of generators having been used in a number of recent studies with model implementations of GPU simulations [11, 13, 16, 35].

3 Multiply with carry

Due to the less than optimal quality of random-number streams generated by LCGs, a number of generalizations and improvements *without* increasing the size of the state have been proposed. One well-known example is the multiply-with-carry approach initially suggested by Marsaglia [36]. In the simplest case, one considers the sequence

$$x_{n+1} = ax_n + c_n \pmod{m},$$

$$c_{n+1} = \lfloor (ax_n + c_n)/m \rfloor.$$

In other words, the additive term c_n in the (n+1)st step is the carry from the previous iteration, hence the name multiply-with-carry (MWC). As for the LCGs, a particularly efficient generator results from taking m to be a multiple of the intrinsic word length. We consider $m=2^{32}$ here, which allows to pack the whole state (x_n, c_n) in a 64-bit integer variable. For suitably chosen a, the period is found to be p=am-2 which, for a only slightly smaller than $m=2^{32}$ comes close to the period $p=2^{64}$ of the 64-bit LCG. A GPU implementation of this generator was originally suggested in the CUDAMCML photon simulator package [24] and was recently used for the Potts model simulations reported in Ref. [14]. 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) [4]. A standard choice for a single generator instance is a=4294967118. Since these conditions on a are sufficiently simple, it is relatively straightforward to produce a large number of multipliers for parallel execution of RNGs with a comparable period and comparable quality of the generated random number streams. (This is in contrast to LCGs, where

Table 1. Internal energy e per spin and specific heat C_V for a 1024×1024 Ising model with periodic boundary conditions at $\beta=0.4$ from simulations on CPU and on GPU using different random number generators. $\Delta_{\rm rel}$ denotes the deviation from the exact result relative to the estimated standard deviation. The columns $t_{\rm up}^{k=1}$ and $t_{\rm up}^{k=100}$ show the average time per spin update in ns for k=1 single and k=100 multi-hit updates, respectively (see text). This test uses about 10^{13} or 2^{43} random numbers.

method	\overline{e}	$\Delta_{ m rel}$	C_V $\Delta_{ m rel}$		$t_{\mathrm{up}}^{k=1}$	$t_{\rm up}^{k=100}$					
exact	1.106079207	0	0.8616983594		ар	чь					
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					

the conditions for full period are more complicated and only a few combinations of parameters produce streams of acceptable quality [2,31].)

We have used the batteries from the TestU01 suite to judge the quality of the pseudo-random sequence produced by a single MWC generator. As is summarized in Table 2 it fares marginally better than a 32-bit LCG but, in fact, worse than the 64-bit LCG considered in the previous section. This is somewhat surprising in view of the fact that this class of generators is often considered superior to LCGs, and the space requirements for (x_n, c_n) is the same as that for the 64-bit LCG. The performance of the well-engineered GPU implementation of Ref. [24] for the pure random-number production comes in at only slightly below that of the 64-bit LCG with around 44×10^9 32-bit random numbers per second on a GTX 480.

As mentioned above, it is possible to systematically generate multipliers by finding the largest safe prime am-1 with a less than 2^{32} (which is just the $a=4\,294\,967\,118$ above) and then systematically working one's way down from there towards smaller multipliers. To check for primality one uses probabilistic tests such as the Rabin-Miller algorithm with parameters that make the occurrence of false positives sufficiently unlikely. There are more than 10^6 such multipliers for $m=2^{32}$, which should be sufficient for most applications. While the efficient generation of large numbers of multipliers is possible using arbitrary-precision libraries such as the GNU Multiple Precision Library, these multipliers need to be transferred to and stored in the GPU main memory, as well as loaded by each independent thread prior to generating random numbers. Hence, as far as memory bandwidth is concerned, it is fair to say that the state of this generator is in fact 64+32=96 bits.

To complement the tests on pure random number generation we also studied the Metropolis simulation of an Ising model as an application benchmark. The corresponding results are collected in Table 1. Comparing the estimates of e and C_V to

the exact results, we find complete statistical consistency in terms of the observed fluctuations. For comparison, we also show the results of using the same multiplier (but different seeds) for each generator instance, which also yields satisfactory results, but this setup is found to yield slightly better performance since the cooperative load operation of the multiplier field is no longer required. The application performance of this generator is very similar to that of the 64-bit LCG, with a moderate overhead seen in the k=1 case for the loading of the extra 32 bit multiplier.

The similar class of subtract-with-borrow algorithms [36] is the basis for the RAN-LUX generator popular in high-energy physics [37]. There, additional skipping in the random-number sequence is used to get rid of the short-ranged correlations. An implementation of this generator on ATI cards was presented in Ref. [27]. It cannot compete in performance, however, with some of the good-quality generators discussed below. Another generalization of the multiply-with-carry generator is possible in the form of a multi-term lagged Fibonacci generator with additional carry. This could be implemented on GPU using state sharing rather similarly to the case of the more standard lagged Fibonacci generators discussed next.

4 Lagged Fibonacci generators

A large number of RNGs with bigger state can be written in the form of a generalized lagged Fibonacci sequence with recursion

$$x_n = a_1 x_{n-1} \otimes a_2 x_{n-2} \otimes \dots \otimes a_k x_{n-k} \pmod{m}. \tag{4}$$

Here, the operator \otimes typically denotes one of the four operations addition +, subtraction -, multiplication * and bitwise XOR \oplus , respectively. Since a history of at least k steps of generated x_n must be kept in memory in order to perform the recursion, this class of generator effectively has state size 32k bits (assuming 32 bit wide variables x_n). In the following, we choose $m=2^{32}$. While generators with $\otimes=+$ are sometimes also known as multiple recursive RNGs, the choice $\otimes=\oplus$ often goes under the name of Tausworthe or shift register generator [2,4]. Here, we concentrate on the most commonly considered case of generators with two terms, i.e., two non-zero multipliers a_r and a_s such that

$$x_n = a_s x_{n-s} \otimes a_r x_{n-r} \pmod{m},$$

which are reminiscent of the Fibonacci series $F_n = F_{n-1} + F_{n-2}$ that led to the name of this class of generators. For an appropriate choice of the multipliers a_s and a_r (as well as the initial values) and assuming r > s, it is possible to achieve periods of $p = 2^r - 1$ for $\otimes = \oplus$, $p = 2^{31}(2^r - 1)$ for $\otimes = \pm$, and $p = 2^{29}(2^r - 1)$ for $\otimes = *$, respectively [19]. If the lag r is big enough, the periods can be made astronomically large. For $\otimes = +$ and r = 1279 considered below, for instance, we have $p = 2^{31}(2^{1278} - 1) \approx 10^{394}$.

As an example of this class of generators discussed in Ref. [25], we consider $\otimes = +$ and use an implementation that works directly on the output variables $u_n \in [0,1]$ by using floating-point arithmetic as

$$u_n = u_{n-r} + u_{n-s} \pmod{1}.$$
 (5)

For good quality one needs $r \gtrsim 100$, leading to relatively large storage requirements, but here the generation of s random numbers can be vectorized by the n threads of a block. Hence, the ring buffer of length r+s 32-bit words is shared among the threads of a block, leading to a state size of (r+s)/n words per thread. If one chooses s only slightly larger than the number of threads per block (and r not too much

larger than s), only a few words per thread are consumed. A number of good choices for the lags r and s are collected in Ref. [19]. As examples, we use here r=521, s=353 and r=1279, s=861, respectively. Since one cannot have a large number of independent, "good" pairs (r,s) resulting in a reasonable state size per thread (assuming a constant number of threads dictated by the application), division into sub-streams is the only possible strategy for achieving independence between the streams generated by different blocks. To this end, one can use a modified skipping procedure similar to that discussed in the context of LCGs as outlined in Ref. [19]. In view of the astronomic period, however, it appears safe to just seed the ring buffers of the generators for different blocks with an independent RNG.

The quality of the thus generated streams of pseudo-random numbers crucially depends on the choice of the lags r and s. For the example generator (5), both choices r = 521 and r = 1279 pass the SmallCrush battery of tests, cf. Table 2. The generator with the smaller lag fails two variants of the gap test in Crush, whereas the choice r = 1279 passes all tests apart from a suspicious result for a random walk test in Crush. In BigCrush, another suspicious result for a random walk test as well as a failed variant of the gap test are found; all other tests are passed. Hence, it is safe to say that from a theoretical perspective these generators produce random streams of satisfactory quality if only r is chosen large enough. Regarding the Ising application test on GPU using random seeding of the initial states of ring buffers for different thread blocks, we find a significant deviation from the exact result for the internal energy for the smaller lag r = 521 and full consistency for the larger lag r = 1279 for the 1024^2 system at $\beta = 0.4$ considered here, cf. the corresponding entries in Table 1. The performance of the generator crucially depends on the number of threads used per block as the number of words per thread (r+s)/n decreases as n < sapproaches s. The performance results in Tables 1 and 2 are for n = 512 threads, which is realistic for the applications considered, but somewhat unfavorable for the r = 1279 generator. The pure RNG peak performance for either choice of r is around 23×10^9 32-bit numbers per second for the GTX 480, about half of the performance of the 64-bit LCG. While these performances are virtually identical for r = 1279 and r = 521, we find that r = 1279 significantly slows down the Ising code as compared to r = 521, see the performance data in Table 1. The performance of the stand-alone generator is also illustrated in Fig. 1 as a function of the number of thread blocks

Improvements of the outlined scheme are easily conceivable. Three-term recurrences, for instance, are known to generate significantly improved random-number streams already at smaller choices of the lags [19]. Alternatively, one might consider using *multiplicative* lagged Fibonacci generators which have been shown to be Crush-resistant [6]. A generator that has been widely used in spin-model simulations, including the simulations carried out on the FPGAs of the Janus special-purpose computer [38], is the following recurrence suggested by Parisi and Rapuano in Ref. [8],

$$x_n = x_{n-24} + x_{n-55},$$

 $u_n = (x_n \oplus x_{n-61})/m,$

with $m=2^{32}$. This corresponds to a lagged Fibonacci generator with an additional shift-register step to improve the quality of the output. For this specific choice of lags, however, we find that the quality of the generated random-numbers streams is relatively poor with two suspicious tests in SmallCrush and 8 failed tests in Crush. In view of these results and the fact that this specific choice of lags does not appear very suitable for vectorization with the number of cores available on the GPUs considered here, we have not attempted a GPU implementation of this specific generator. Another popular generator, suggested in Ref. [39] and dubbed RANMAR, consists of

the combination of a two-term lagged Fibonacci and a second, arithmetic sequence. While good at its time, it fails a number of tests already in smaller suites (partially due to the low resolution of 24 bits) and is hence probably not appropriate any more for today's applications. A GPU implementation of RANMAR on ATI cards has been discussed in Ref. [27].

5 Mersenne twister

The very popular Mersenne twister generator [21] is based on a variant of the general lagged Fibonacci generator concept outlined in the previous section in the form of a twisted generalized feedback shift register generator. For the case of 32-bit numbers, one chooses a Mersenne prime $2^k - 1$ and sets $N = \lceil k/32 \rceil$. The generator is then based on the recursion

$$x_n = (x_{n-N}|x_{n-N+1})A \oplus x_{n-N+M}. (6)$$

Here, 1 < M < N is the additional, smaller lag and $(x_{n-N}|x_{n-N+1})$ denotes the concatenation of the 32-r most significant bits of x_{n-N} with the r least significant bits of x_{n-N+1} , where r=32N-k. The 32×32 bit-matrix A defines the twist operation which is chosen in a specifically simple form that allows for an efficient implementation in terms of shift operations. To improve the equidistribution properties, the sequence x_n is subjected to an additional tempering transformation, such that the output sequence finally is

$$u_n = |x_n T|,$$

where the tempering bit-matrix T is a suitably chosen combination of single-term shifts and binary-and operations, see Ref. [21] for details. It can be shown that, if the corresponding characteristic polynomial is primitive, this class of generators achieves the maximal period of $p=2^k-1$ [21]. The most popular choice is MT19937 with k=19937, leading to N=624 and r=31 with the additional lag M=397. The period is maximal with $p=2^{19937}-1\approx 4\times 10^{6001}$. While the quality of these generators is generally good, they systematically fail tests in the Crush suites related to \mathbb{F}_2 linearity.

Without the use of state sharing, implementations of this type of generator lead to very large states, such that they are not suitable for the type of simulations discussed here. A smaller version of Mersenne twister with k = 607 and hence state size of $\lceil 607/32 \rceil = 19$ 32-bit words using an independent generator instance for each thread has been part of the NVIDIA CUDA SDK for some time. This is still significantly in excess of the (arbitrary) cut-off of 4 words per thread adopted here. Due to the reduced state size and period, this generator fails some random-walk tests in addition to the routines based on \mathbb{F}_2 linearity [26]. A variant of the Mersenne twister more suitable for GPUs has been suggested in Ref. [26]. It uses state sharing and a somewhat different transformation particularly suitable for GPU characteristics. Vectorization is performed along the same lines as outlined above for the Fibonacci generator, generating N-M numbers in one parallel sweep. The choice of the Mersenne prime $2^{11213} - 1$ favored in Ref. [26] leads to N = 351 which, ensuring M < 95, allows for 256 threads to generate numbers simultaneously. The resulting state size is hence 351/256 < 2 words per thread plus the overhead for the transformation parameters common to each thread block. This adapted generator, dubbed MTGP, has been included in the NVIDIA cuRAND library of random-number generators starting with version 4.1 [22]

The Mersenne twister generator can be run with parameter sets chosen such that distinct instances have distinct irreducible characteristic polynomials of the transition function, at least making it plausible that these sequences are uncorrelated [26].

To this end, a 16-bit ID is used as an input to a separate, number-theoretic code that searches for an appropriate parameter set. It is, however, not guaranteed that such a set of parameters can be found. For MTGP, a different approach with 32-bit IDs is used which, however, does not guarantee to generate distinct characteristic polynomials [26]. While this setup, in principle, allows for a large number of parallel instances, the parameter search is found to be very time consuming such that, for instance, finding a single parameter set for k=11213 can take up to an hour on current hardware [26]. As a consequence, cuRAND comes with a built-in set of 64 (presumably) independent sequences — far too few for many of the applications we are discussing here. Another inflexibility comes through the restriction to 256 threads per block which cannot be easily changed.

We have only benchmarked the MTGP code here, finding that it fails, as expected, those tests in BigCrush based on \mathbb{F}_2 linearity. The performance is found to be at an acceptable, but not outstanding 18×10^9 32-bit random-number samples per second. As the implementations available in CUDA 4.1 (which is still incomplete) and Saito's website are limited to 200 parameter sets, while our Ising test uses 2048 blocks, in view of the expensive parameter search mentioned above we have not attempted the Ising test here.

6 XORShift generators

Another class of generators proposed by Marsaglia [30] is based on the observation that the XORShift operation, i.e., the binary XOR between a word and a shifted version of itself, can be performed very fast on modern computers as it does not involve integer addition, multiplication or division, and it leads to high-quality pseudorandom sequences. Representing a word of size w as a vector of bits $x = (x_1, \ldots, x_w) \in \{0,1\}^w$, a left shift can be expressed as a matrix multiplication $(x_1, \ldots, x_W)L = (x_2, \ldots, x_W, 0)$ with the left shift matrix

$$L = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 \end{pmatrix}. \tag{7}$$

If we denote by I the identity matrix, an XORShift by a positions can be written as $x(I \oplus L^a)$, which corresponds, in C programming language, to the expression $x \land (x \lessdot a)$. The recursion suggested in Ref. [30] consists of three shifts,

$$x_n = x_{n-1}(I \oplus L^a)(I \oplus R^b)(I \oplus L^c) =: x_{n-1}M,$$
 (8)

where $R=L^T$ denotes the right shift and a word-size w of 32 or 64 bits is used. For an appropriate choice of the shifts a,b and c, namely when the characteristic polynomial $P(z)=\det(M-zI)$ is primitive, these generators attain maximal period 2^w-1 . While, for w=32 or w=64, this is still rather low, similar transition matrices for w=96, w=128 and w=160 are also suggested [30]. The combination of the w=160 bit flavor with a 32-bit Weyl generator (see below) defines the XORWOW RNG implemented in the cuRAND library [22]. While this has reasonably good properties (including a period of $2^{192}-2^{32}$), the state of 192 bits per thread is larger than desirable. Panneton et~al.~[40] criticized Marsaglia's generators for poor quality and tried to amend them by including more than three distinct shift operations. Brent $[41]^1$ instead concentrated on finding good parameter sets, for multiple recursive generators, i.e. (a,b,c) for the above generator, by the use of heuristics.

Also note the summary at http://papercore.org/Brent2007.

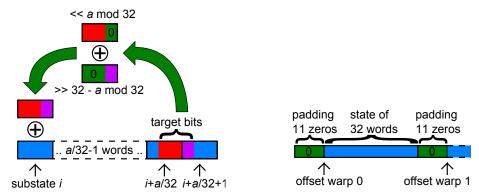


Fig. 2. Left: left shift on a shared memory array, which stores the state of a RNG. For thread i to update its part of the state, it needs a region of the state that spans the sub-states of threads i + a/32 and i + a/32 + 1. Right: Padding of the state array in shared memory. Zeros are placed in between the states of different warps to avoid the need for treating shifts crossing the state boundary separately.

As a more space efficient approach than XORWOW with even better statistical properties, we here suggest to use the three-shift generator (8), but for a dramatically increased word size of w = 1024 bits. Adopting Brent's heuristics [41], we performed a search for a generator with maximal period $2^{1024} - 1$ using Sage [42] (and particularly the included library NTL [43]). We found a generator with the parameters a = 329, b = 347, and c = 344, which has a primitive characteristic polynomial of weight² 475. This generator is implemented on GPU by splitting the 1024 bits of state into a single WORD=32-bit word in each of the WARPSIZE=32 threads of a warp and using the threads of a warp to cooperatively update the 1024-bit state. The XORShifts are then performed in the following way. Consider, for instance, a left shift by a bits as illustrated in the left panel of Fig. 2. The bits arriving at the part of the state at thread i originate from the most significant bits of the word of thread $i + \lfloor a/32 \rfloor$ and the least significant bits of the word of thread i + |a/32| + 1. These parts need to be shifted left and right, respectively, to be assembled to the updated word at position i. Our full CUDA implementation is shown in Listing 1. There, NWARPS denotes the number of warps per block and the type state_t is simply an unsigned integer. This implementation benefits from the fact that all three shifts correspond to a WORDSHIFT= $\lfloor a/32 \rfloor$ of 10, leading to RAND_A = a (mod 32) = 9 and accordingly RAND_B = 27 and RAND_C = 24. Though shifts exceeding the word-size could be taken care of using conditionals, we prefer to simply pad the shared array with WORDSHIFT+1 words of zeros as shown in the right panel of Fig. 2. As the threads of a warp are always in sync, explicit synchronization is not needed. However the shared array has to be marked as volatile to make sure the compiler writes all values to shared memory and does not simply keep them in registers instead³.

Listing 1. Kernel XORShift.

```
1 /*
2 * Updates the RNG state in cooperation with in-warp neighbors.
3 * Uses a block of shared memory of size
```

 $^{^{2}\,}$ The weight of a polynomial is the number of non-zero terms.

³ Note that the very recently released version 4.2 of the CUDA toolkit allows for a direct exchange of data between threads within a warp using so-called "warp shuffle" functions. Using this feature for implementing the present generator would clearly free shared memory for other uses and, presumably, increase the overall performance.

```
* (WARPSIZE + WORDSHIFT + 1) * NWARPS + WORDSHIFT + 1.
   * Parameters:
     state: RNG state
     tid: thread index in block
     stateblock: shared memory block for states
   * Returns:
     updated state
10
11
12 __device__ state_t rng_update(state_t state, int tid,
                                 volatile state_t* stateblock)
14 {
16 /* Indices. */
int wid = tid / WARPSIZE; // Warp index in block
18 int lid = tid % WARPSIZE; // Thread index in warp
19 int woff = wid * (WARPSIZE + WORDSHIFT + 1) + WORDSHIFT + 1;
                                                      // warp offset
21 /* Shifted indices. */
22 int lp = lid + WORDSHIFT; // Left word shift
23 int lm = lid - WORDSHIFT; // Right word shift
25 /* << A. */
26 stateblock[woff + lid] = state; // Share states
27 state ^= stateblock[woff + lp] << RAND_A; // Left part
28 state ^= stateblock[woff + lp + 1] >> WORD - RAND_A; // Right part
30 /* >> B. */
stateblock[woff + lid] = state; // Share states
32 state ^= stateblock[woff + lm - 1] << WORD - RAND_B; // Left part
33 state ^= stateblock[woff + lm] >> RAND_B; // Right part
35 /* << C. */
36 stateblock[woff + lid] = state; // Share states
37 state ^= stateblock[woff + lp] << RAND_C; // Left part
38 state ^= stateblock[woff + lp + 1] >> WORD - RAND_C; // Right part
40 return state;
41 }
```

In view of the large period of the generator, we use skip-ahead to partition the sequence into substreams to be used by different warps. For this purpose, we decided to split the whole random number sequence into blocks of $2^{137}\approx 2\times 10^{41}$ numbers, assigning them successively to the instances. With current hardware, it appears impossible for any of the instances to exhaust their sub-sequences. To this end, we let all warps start with the same state and have them skip the appropriate number of update steps by multiplying the state with the precomputed 2^{137} -th power of the recursion matrix M. The matrix, included in a header, is copied to the device and bound to a texture to perform a matrix multiplication. Starting from the resulting states after this initialization the warps can simply continue to update normally as shown in the previous section. If a large number of instances is seeded, we found that this approach leads to very long kernel running times, which can lead to problems if the used GPU is concurrently used for display purposes as well. Such problems can be avoided by including higher powers of the block skip matrix to reduce the number of multiplications needed. An alternative, more sloppy approach consists of simply

seeding each generator instance with another RNG which, in view of the large period, should also prevent any overlapping of sequences for all practical purposes.

Similar to the approach suggested in Ref. [30], we also considered a combination of the XORShift generator with a simple Weyl sequence,

$$y_n = (y_{n-1} + c) \mod 2^w, \tag{9}$$

with an odd constant c. As for XORWOW, we chose w=32 and $c=362\,437$ and, following Brent [41], return $y_n^i(I\oplus R^\gamma)+x_n^i\pmod{2^w}$, where the superscript i refers to the local state of thread i and $\gamma=w/2$. The period of the resulting generator is thus increased to $(2^{1024}-1)2^{32}$. Brent argues that in the XORShift generator elements with low Hamming weight (i.e., small numbers of non-zero bits) will be followed by other low weight elements. For our generator with w=1024, the probability for such events is, however, astronomically small. Still, since the extra cost of the outlined combination with a Weyl sequence is relatively small, we include it for the measurements and tests reported below. The calculation of any state of the Weyl generator is trivially possible in one step,

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

such that there is no need to store the state in memory in between invocations⁴.

To assess the statistical quality of the resulting random-number sequence, we subjected it to the batteries in the TestU01 suite. These tests were performed for two orders of the generated numbers, namely (a) single-thread order, feeding the sequence generated by a single thread to the test, and (b) warp order, feeding the 32 numbers generated by each warp in one step sequentially to the test. In both cases, we found that all tests were passed. In addition, we tested for equidistribution directly. If we take output values u_n of our generator, we expect them to fill the interval [0,1) uniformly. Thus if we divide the interval into 2^l cells, each cell should be hit the same number of times. More generally, vectors made of t successive numbers should evenly fill the $[0,1)^t$ hypercube. We implemented these tests as described in Ref. [40], finding acceptable uniformity. As discussed by Panneton [40], there are different choices of the matrix M in Eq. (8) leading to the same characteristic polynomial. Of the four possible choice, we found one with rather bad equidistribution properties with the other three being acceptable, and our choice being the best of the available options.

In terms of performance, we find the standalone generator to produce a good 18×10^9 uniform 32-bit random-numbers per second⁵. As expected from the statistical testing, the Ising application test does not reveal any significant deviations from the exact results, see the corresponding data in Table 1. The performance in the single-hit and multi-hit versions of the Ising application is reasonably good, benefiting from the small state and arithmetic simplicity of the generator. The source code of this generator is included for future reference in the Supplementary Material of this review article.

7 Counter-based generators

The essential complication of parallelizing random-number generators is rooted in the fact that they are inherently recursive and thus appear to be, at first sight, intrinsically serial. Also, it is this recursion that necessitates to store a generator state in between

⁴ Note that the seed of the Weyl generator is the same for all instances since the chosen size 2^{137} of sub-streams is a multiple of the Weyl generator's period 2^{32} .

 $^{^{5}}$ Somewhat better results are found for version 4.1 of the CUDA Toolkit.

Table 2. Overview of GPU random-number generators discussed in this review. 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. Note that the Philox generators, albeit occupying local memory of 4×32 bits for number generation, do not require to transfer a "state" from and to global memory as long as the generator keys are deduced from intrinsic variables such as particle numbers etc.

generator	bits/thread	failu	res in Tes	Ising test	perf.	
	•	SmallCrus	h Crush	BigCrush		$\times 10^9/\mathrm{s}$
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

invocations (and, therefore, uses up precious bandwidth for loads and stores). The extremely simple Weyl generator discussed in the previous section appears to be a notable exception as the one-step expression $y_n = (y_0 + nc) \mod 2^w$ is of the form

$$x_n = f_k(n), (10)$$

that is, the nth number in the sequence is determined directly by applying some function f_k to the integer n itself, which therefore acts as a counter. Here, k is interpreted as a key representing all or part of the parameters such as y_0 , c and w for the Weyl sequence. Note that if n is a w-bit counter and f_k is a bijection, the period of this type of generator is 2^w . While the Weyl generator itself certainly is not good enough as a RNG meeting today's standards, one might wonder whether there are better generators based on the same idea. A number of functions designed along these lines have been recently discussed by Salmon $et\ al.$ in Ref. [20].

While such generators have not received much attention in the past for use in simulations, they are very alike to the functions used in secret-key cryptography. There, one has a family of encryption functions that depend on a key k and encode the plain-text n (represented as an integer) into a cipher-text x_n (encoded as another integer) [44]. This is clearly of the form (10), assuming that f_k is a bijection allowing to uniquely decode the cipher-text. The connection to random-number generation comes in through the security requirements of such function sets f_k in cryptographic applications: if the cipher-texts contain any structure that allow to distinguish them from pure random sequences, this is a weakness of the system potentially allowing to break the code (i.e., to find the key or plain-text only knowing the cipher-text). It is therefore well-known in the cryptographic community that established systems such as DES (the data encryption standard) and AES (the advanced encryption standard) can be viewed as extremely high-quality random-number generators [45].

AES is an iterative block cipher based on the repeated application of keyed bijections in several rounds designed to ensure diffusion of bits, i.e., generation of highly random output from highly regular inputs. It uses a so-called substitutionpermutation network, which applies repeated substitutions (S-boxes) and permutations (P-boxes) to the bits of the chosen block of the plain-text. The resulting bijections are highly non-linear, in contrast to most of the transformations used in traditional RNGs. The block size in AES is 128 bits, leading to a more than sufficient period of $2^{128} \approx 3 \times 10^{38}$. For details of the AES transformation see, e.g., Ref. [44]. The authors of Ref. [20] implemented AES as an RNG on CPU (there using the hardware support for AES built into recent Intel and AMD CPUs) and GPU. These techniques produce pseudo-random sequences passing all tests, but they are relatively slow unless the mentioned special-purpose hardware support is available (which is not the case on current GPUs).

To provide faster generators without hardware support, Salmon *et al.* suggest a simplified schedule based on cryptographic techniques. The core component is based on integer division and its remainder,

$$\mathrm{mulhi}(a, b) = \lfloor (a \times b)/2^w \rfloor,$$

$$\mathrm{mullo}(a, b) = (a \times b) \mod 2^w,$$

which can be performed efficiently on most architectures (often reducing to one machine instruction). The main iteration (or S-box) picks two words (L,R) out of a block of N words of w bits and computes

$$L' = \text{mullo}(R, M),$$

 $R' = \text{mulhi}(R, M) \oplus k \oplus L.$

The final output is the result of r rounds (so-called Feistel iterations) of the application of N/2 such S-boxes with different multipliers M but, for each thread, constant "key" k. For N>2, the N elements are additionally permuted in between rounds (P-boxes). Since multiplication, permutation and XOR \oplus are bijective, it is clear that the transformation is bijective. The quality of the resulting class of generators, dubbed Philox-Nxw_r, can be systematically improved by increasing the number r of Feistel iterations. The authors of Ref. [20] empirically find that $r \geq 7$ is required for N=4 and w=32 to achieve Crush-resistance.

We tested the generators Philox-4x32_7 and Philox-4x32_10 on GPU. Note that, although this generator requires local storage for four 32-bit words (128 bits) for performing the iterations, it does not require to load or store a state, such that its storage requirement is of a different nature than those of the recursive generators. The use of four words leads to a period of 2^{128} . Since such (pseudo-)cryptographic bijections are designed to deliver outputs essentially indistinguishable from random sequences for any choice of k, different keys can be used to generate independent random-number streams in parallel simulations. For the 64-bit key used here, this allows to generate 2⁶⁴ independent random-number sequences, ideal for the parallel applications considered here. Since the key and sequence space can be partitioned arbitrarily, it is straightforward to use intrinsic logical variables to determine the random numbers to be used. In a parallel Monte Carlo simulation, therefore, the counter could correspond to an iteration or sweep number, whereas the key might be chosen to represent the particle/spin number and further parameters (temperature, disorder realization, system size, ...) characterizing the whole run. Using intrinsic variables for sub-stream selection has the additional advantage of producing identical results for any specific execution configuration on GPU or even between CPU and GPU implementations.

The random-number streams of these generators have already been tested in various sample-orders against the batteries in TestU01 in Ref. [20] and were found to pass all tests. In addition to that, we used the Ising application test and found no

deviations, cf. the data in Table 1. Regarding execution speed, we find the standalone generators to perform at 30×10^9 for r=10 and 41×10^9 for r=7, which is better than the other high-quality generators considered here. Similarly, in the Ising test the Philox performance is rather good. Note that Philox4x32 produces four 32-bit random numbers per invocation. For the Ising simulation with k=1, however, each thread only consumes two numbers such that the k=1 performance results are, in fact, disfavoring Philox and could be improved by rearranging the code accordingly. For k=2, were all produced random numbers are also consumed, Philox4x32_7 results in 0.1379 ns per attempted spin flip compared to 0.1278 ns for the LCG32 and 0.1330 for LCG64.

8 Conclusions

The generation of high-quality random numbers is an issue of continuing interest for those engaging in computer simulation studies. After a number of unpleasant surprises in the early years [7,8], the community has today at its disposal a number of generators with very long periods and passing most statistical tests for simulations on serial machines such as single CPUs. With the advent of massively parallel machines (some of the current clusters already have a total of more than 1 million GPU cores), the search for adaptations of proved generators or the invention of entirely new RNGs has begun. Apart from the more general problem of parallel computing to provide an exceedingly large number of independent random-number streams, simulations on GPU are faced with the additional challenge of finding generators with small state or with the possibility of flexible state sharing between the threads of a block (or warp) to accommodate the small amount of memory local to the multiprocessors and the memory bandwidth limitations.

Simple, small-state generators such as linear congruential or multiply-with-carry variants can be very fast. The statistical quality of the resulting sequences, however, is not ideal for high-precision applications. State sharing, allowing generators with larger states and hence much longer periods and ensuing better statistical quality of produced numbers, appears to be a much more promising strategy, providing some generators passing all tests of the extensive TestU01 suite. We suggest a new generator along these lines, based on the XORShift idea proposed by Marsaglia [30], which passes all tests and provides very good performance. For some generators of this type, such as the Mersenne twister for graphics processors suggested in Ref. [26] and included in the latest version of the cuRAND library, however, generation of appropriate parameter sets for a large number of parallel instances is a challenging problem in itself. A completely different approach [20] based on the keyed bijections used in symmetric-key cryptosystems is very versatile in producing large numbers of independent random-number streams, does not require to save a state by coupling keys and counters to intrinsic variables such as particle numbers and additionally provides one of the most performant high-quality generators currently available on GPUs.

Acknowledgments

M.W. thanks W. Peterson for bringing Ref. [20] to his attention. M.W. acknowledges support by the DFG under contract No. WE4425/1-1 (Emmy Noether Programme).

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