

SPRNG: A SCALABLE LIBRARY FOR PSEUDORANDOM NUMBER GENERATION

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In this article we outline some methods for parallel pseudorandom number generation. We will focus on methods based on parameterization, meaning that we will not consider splitting methods. We describe parameterized versions of the following pseudorandom number generators: (i) linear congruential generators, (ii) shift-register generators, and (iii) lagged-Fibonacci generators. We briefly describe the methods, detail some advantages and disadvantages of each method and recount results from number-theory that impact our understanding of their quality in parallel applications. Finally, we present a short description of a scalable library for pseudorandom number generation, called SPRNG. The description contained within this document is meant only to outline the rationale behind and the capabilities of SPRNG. Much more information, including examples and detailed documentation aimed at helping users with putting and using SPRNG on scalable systems is available at the URL: <http://www.ncsa.edu/Apps/SPRNG>.

1 Introduction

Monte Carlo applications are widely perceived as embarrassingly parallel. The truth of this notion depends, to a large extent, on the quality of the parallel random number generators used. It is widely assumed that with N processors executing N copies of a Monte Carlo calculation, the pooled result will achieve a variance N times smaller than a single instance of this calculation in the same amount of time. This is true only if the results in each processor are statistically independent. In turn, this will be true only if the streams of random numbers generated in each processor are independent.

We briefly present several methods for parallel pseudorandom number generation and discuss pros and cons for each method. If the reader is interested in background material on plain old serial pseudorandom number generation in general, consult the following references by Knuth¹², L'Ecuyer¹⁴, Niederreiter³¹, and Park and Miller³², while a good overview of parallel pseu-

¹⁰Monte Carlo enthusiasts prefer the term "naturally parallel" to the somewhat derogatory "embarrassingly parallel" coined by computer scientists.

dorandom number generation can be found in a recent work by the present article's author²⁶.

In our parallel pseudorandom number generation review we are interested, exclusively, with methods for obtaining parallel pseudorandom number generators (PPRNGs) via parameterization. The exact meaning of parameterization depends on the type of PRNG under discussion, but we wish to distinguish parameterization from splitting methods. We will not be considering the production of parallel streams of pseudorandom numbers by taking substreams from a single, long-period PRNG. For readers interested in splitting methods and the consequences of using split streams in parallel please consult the works by Deák⁵, De Matteis and Pagnutti^{7,8,9}, Frederickson *et al.*¹⁰, and L'Ecuyer and Gôlé¹⁵. In general, we seek to determine a parameter in the underlying recursion of the PRNG that can be varied. Each valid value of this parameter will lead to a recursion that produces a unique, full-period stream of pseudorandom numbers. We then discuss efficient means to specify valid parameter values and consider these choices in terms of the quality of the pseudorandom numbers produced.

The plan of the paper is as follows. In §2 we present an extensive overview of parallel pseudorandom number generation mostly viewed from the parameterization point of view. In §2.1 two methods for parameterizing linear congruential generators (LCGs). In §2.2 we present a parameterization of another linear method: shift-register generators (SRGs). This parameterization is analogous to one of the LCG parameterizations presented in §2.1. In §2.3 we consider the parallel parameterization of so-called lagged-Fibonacci generators. In §3, we present the Scalable Parallel Random Number Generators (SPRNG) library, a comprehensive tool for parallel and distributed pseudorandom number generation developed by the author. Finally in §4 we discuss open problems, and provide concluding remarks.

2 Parallel Pseudorandom Number Generation

In this next, rather extensive, section we will look at several methods for parallel pseudorandom number generation. Most of the methods we will present will be based on some kind of parameterization of the generators.

2.1 Linear Congruential Generators

The most commonly used generator for pseudorandom numbers is the LCG. The LCG was first proposed for use by Lehmer¹⁶, and is referred to as the Lehmer generator in the early literature. The linear recursion underlying

LCGs is:

$$x_n = ax_{n-1} + b \pmod{m}. \quad (1)$$

When the multiplier, a , additive constant, b , and modulus, m , are chosen appropriately one obtains a purely periodic sequence with period as long as $\text{Per}(x_n) = 2^k$, when m is a power-of-two, and $\text{Per}(x_n) = m - 1$, when m is prime. It is well known that s -tuples made up from LCGs lie on lattices composed of a family of parallel hyperplanes, Marsaglia²¹. The x_n 's in Eq. (1) are integer residues modulo m , and a uniform pseudorandom number in $[0, 1]$ is produced via $z_n = x_n/m$, and the initial value of the LCG, x_0 , is often called the seed.

The most important parameter of an LCG is the modulus, m . Its size constrains the period, and for implementational reasons it is always chosen to be either prime or a power-of-two. Based on which type of modulus is chosen, there is a different parameterization method. When m is prime, a method based on using the multiplier, a , as the parameter has been proposed. The rationale for this choice is outlined in Mascagni²⁵, and leads to several interesting computational problems.

2.1.1 Prime Modulus

Given we wish to parameterize a when m is prime we must determine first the family of permissible a 's. A condition on a when m is prime to obtain the maximal period (of length $m - 1$ in this case) is that a must be a primitive element modulo m , Knuth¹². Given primitivity, one can use the following fact: if a and α are primitive elements modulo m then $\alpha = a^i \pmod{m}$ for some i relatively prime to $\phi(m)$. Note that when m is prime that $\phi(m) = m - 1$. Thus a single, reference, primitive element, a , and an explicit enumeration of the integers relatively prime to $m - 1$ furnish an explicit parameterization for the j th primitive element, a_j as $a_j = a^{i_j} \pmod{m}$ where i_j is the j th integer relatively prime to $m - 1$. Given an explicit factorization of $m - 1$, Brillhart *et al.*³, efficient algorithms for computing i_j can be found in a recent work of the author²⁵. However, two important open questions remain: (1) is it more efficient overall to choose m to be amenable to fast modular multiplication or fast calculation of the j th integer relatively prime to $m - 1$, and (2) does the good interstream correlation mentioned in Mascagni²⁵ also ensure good intrastream independence via the spectral test? The first of these questions is of practical interest to performance, the

³An integer, a , is primitive modulo m if the set of integers $\{a^i \pmod{m} | 1 \leq i \leq m - 1\}$ equals the set $\{1 \leq i \leq m - 1\}$.

second, however, if answered negatively, makes such techniques less attractive for parallel pseudorandom number generation.

2.1.2 Power-of-two Modulus

An alternative way to use LCGs to make a PPRNG is to parameterize the additive constant in Eq. (1) when the modulus is a power-of-two, i.e., to $m = 2^k$ for some integer $k > 1$. This is a technique first proposed by Percus and Kalos³³, to provide a PPRNG for the NYU Ultracomputer. It has some interesting advantages over parameterizing the multiplier; however, there are some considerable disadvantages in using power-of-two modulus LCGs.

The parameterization chooses a set of additive constants $\{b_j\}$ that are pairwise relatively prime, i.e. $\text{gcd}(b_i, b_j) = 1$ when $i \neq j$. A prudent choice is to let b_j be the j th prime. This both ensures the pairwise relative primality and is the largest set of such residues. With this choice certain favorable interstream properties can be theoretically derived from the spectral test³³. However, this choice necessitates a method for the difficult problem of computing the j th prime. In their paper, Percus and Kalos do not discuss this aspect of their generator in detail, partly due to the fact that they expect to provide only a small number of PRNGs. When a large number of PPRNGs are to be provided with this method, one can use fast algorithms for the computation of $\pi(x)$, the number of primes less than x , Deleglise and Rivat⁶, Lagarias, Miller, and Odlyzko¹³. This is the inverse of the function which is desired, so we designate $\pi^{-1}(j)$ as the j th prime. The details of such an implementation need to be specified, but a very related computation for computing the j th integer relatively prime to a given set of integers is given in Mascagni²⁵. It is believed that the issues for computing $\pi^{-1}(j)$ are similar.

One important advantage of this parameterization is that there is an interstream correlation measure based on the spectral test that suggests that there will be good interstream independence. Given that the spectral test for LCGs essentially measures the quality of the multiplier, this sort of result is to be expected. A disadvantage of this parameterization is that to provide a large number of streams, computing $\pi^{-1}(j)$ will be necessary. Regardless of the efficiency of implementation, this is known to be a difficult computation with regards to its computational complexity. Finally, one of the biggest disadvantages to using a power-of-two modulus is the fact the least significant bits of the integers produced by these LCGs have extremely short periods. If $\{x_n\}$ are the residues of the LCG modulo 2^k , with properly chosen parameters, $\{x_n\}$ will have period 2^k . However, $\{x_n \pmod{2^j}\}$ will have period 2^j for all integers $0 < j < k$, Knuth¹². In particular, this means the least-significant

bit of the LCG with alternate between 0 and 1. This is such a major short coming, that it motivated us to consider parameterizations of prime modulus LCGs as discussed in §2.1.1.

2.2 Shift-Register Generators

Shift register generators (SRGs) are linear recursions modulo 2, see Golomb ¹¹, Lewis and Payne ¹⁷, and Tausworthe ³⁵, of the form:

$$x_{n+k} = \sum_{i=0}^{k-1} a_i x_{n+i} \pmod{2}, \quad (2)$$

where the a_i 's are either 0 or 1. An alternative way to describe this recursion is to specify the k th degree binary characteristic polynomial, see Lidl and Niederreiter ¹⁸:

$$f(x) = x^k + \sum_{i=0}^{k-1} a_i x^i \pmod{2}. \quad (3)$$

To obtain the maximal period of $2^k - 1$, a sufficient condition is that $f(x)$ be a primitive k th degree polynomial modulo 2. If only a few of the a_i 's are 1, then Eq. (2) is very cheap to evaluate. Thus people often use known primitive trinomials to specify SRG recursions. This leads to very efficient, two-term, recursions.

There are two ways to make pseudorandom integers out of the bits produced by Eq. (2). The first, called the digital multi-step method, takes successive bits from Eq. (2) to form an integer of desired length. Thus, with the digital multi-step method, it requires n iterations of Eq. (2) to produce a new n -bit pseudorandom integer. The second method, called the generalized feedback shift-register, creates a new n -bit pseudorandom integer for every iteration of Eq. (2). This is done by constructing the n -bit word from x_{n+k} and $n-1$ other bits from the k bits of SRG state. While these two methods seem different, they are very related, and theoretical results for one always hold for the other. One way to parameterize SRGs is analogous to the LCG parameterization discussed in §2.1.1. There we took the object that made the LCG full-period, the primitive root multiplier, and found a representation for all of them. Using this analogy we identify the primitive polynomial in the SRG as the object to parameterize. We begin with a known primitive polynomial of degree k , $p(x)$. It is known that only certain decimations of the output of a maximal-period shift register are themselves maximal and unique with respect to cyclic reordering, see Lidl and Niederreiter ¹⁸. We seek to identify those.

The number of decimations that are both maximal-period and unique when $p(x)$ is primitive modulo 2 and k is a Mersenne exponent is $\frac{2^k-2}{k}$. If a is a primitive root modulo the prime $2^k - 1$, then the residues $a^i \pmod{2^k - 1}$ for $i = 1$ to $\frac{2^k-2}{k}$ form a set of all the unique, maximal-period decimations. Thus we have a parameterization of the maximal-period sequences of length $2^k - 1$ arising from primitive degree k binary polynomials through decimations.

The entire parameterization goes as follows. Assume the k th stream is required, compute $d_k \equiv a^k \pmod{2^k - 1}$ and take the d_k th decimation of the reference sequence produced by the reference primitive polynomial, $p(x)$. This can be done quickly with polynomial algebra. Given a decimation of length $2k + 1$, this can be used as input the Berlekamp-Massey algorithm to recover the primitive polynomial corresponding to this decimation. The Berlekamp-Massey algorithm finds the minimal polynomial that generates a given sequence, see Massey ²⁹ in time linear in k .

This parameterization is relatively efficient when the binary polynomial algebra is implemented correctly. However, there is one major drawback to using such a parameterization. While the reference primitive polynomial, $p(x)$, may be sparse, the new polynomials need not be. By a sparse polynomial we mean that most of the a_i 's in Eq. (2) are zero. The cost of stepping Eq. (2) once is proportional to the number of non-zero a_i 's in Eq. (2). Thus we can significantly increase the bit-operational complexity of a SRG in this manner. The fact that the parameterization methods for prime modulus LCGs and SRGs are so similar is no accident. Both are based on maximal period linear recursions over a finite field. Thus the discrepancy and exponential sum results for both the types of generators are similar, see Niederreiter ³¹.

2.3 Lagged-Fibonacci Generators

In the previous sections we have discussed generators that can be parallelized by varying a parameter in the underlying recursion. In this section we discuss the additive lagged-Fibonacci generator (ALFG): a generator that can be parameterized through its initial values. The ALFG can be written as:

$$x_n = x_{n-j} + x_{n-k} \pmod{2^m}, \quad j < k. \quad (4)$$

In recent years the ALFG has become a popular generator for serial as well as scalable parallel machines, see Makino ²⁰. In fact, the generator with $j = 5$, $k = 17$, and $m = 32$ was the standard PPRNG in Thinking Machines Connection Machine Scientific Subroutine Library. This generator has become popular for a variety of reasons: (1) it is easy to implement, (2) it is cheap to compute using Eq. (4), and (3) the ALFG does well on standard statistical

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tests, see Marsaglia 23.

An important property of the ALFG is that the maximal period is $(2^k - 1)2^{m-1}$. This occurs for very specific circumstances, Brent 2 and Marsaglia and Tsay 24, from which one can infer that this generator has $2^{(k-1) \times (m-1)}$ different full-period cycles, Mascagni *et al.* 27. This means that the state space of the ALFG is toroidal, with Eq. (4) providing the algorithm for movement in one of the torus dimension. It is clear that finding the algorithm for movement in the other dimension is the basis of a very interesting parameterization. Since Eq. (4) tells us how to cycle over the full period of the ALFG, one must find a seed that is not in a given full-period cycle to move in the second dimension. The key to moving in this second dimension is to find an algorithm for computing seeds in any given full-period cycle.

A very elegant algorithm for movement in this second dimension is based on a simple enumeration as follows. One can prove that the initial seed, $\{x_0, x_1, \dots, x_{k-1}\}$, can be bit-wise initialized using the following template:

$$\begin{array}{c|c}
 \text{m.s.b.} & \text{l.s.b.} \\
 \hline
 b_{m-1} & b_0 \\
 b_{m-2} & \dots \\
 \vdots & \vdots \\
 0 & 0 \\
 \vdots & \vdots \\
 0 & 0 \\
 \vdots & \vdots \\
 1 & 1 \\
 x_0 & x_1
 \end{array} \quad (5)$$

Here each square is a bit location to be assigned. Each unique assignment gives a seed in a provably distinct full-period cycle, Mascagni *et al.* 27. Note that here the least-significant bits, b_0 are specified to be a fixed, non-zero, pattern. If one allows an $O(k^2)$ precomputation to find a particular least-significant-bit pattern then the template is particularly simple:

$$\begin{array}{c|c|c}
 \text{m.s.b.} & & \text{l.s.b.} \\
 \hline
 b_{m-1} & b_{m-2} \dots b_1 & b_0 \\
 \hline
 \blacksquare & \blacksquare \dots \blacksquare & \blacksquare \\
 \blacksquare & \blacksquare \dots \blacksquare & \blacksquare \\
 \vdots & \vdots & \vdots \\
 \blacksquare & \blacksquare \dots \blacksquare & \blacksquare \\
 \vdots & \vdots & \vdots \\
 0 & 0 \dots 0 & 1 \\
 x_0 & & x_1
 \end{array} \quad (6)$$

Given the elegance of this explicit parameterization, one may ask about the exponential sum correlations between these parameterized sequences. It is known that certain sequences are more correlated than others as a function of

the similarity in the least-significant bits in the template for parameterization, Mascagni *et al.* 28. However, it is easy to avoid all but the most uncorrelated pairs in a computation, Pryor *et al.* 34. In this case there is extensive empirical evidence that the full-period exponential sum correlation between streams is $O(\sqrt{2^k - 1})2^{m-1}$, the square root of the full-period. This is essentially optimal. Unfortunately, there is no analytic proof of this result, and improvement of the best known analytic result, Mascagni *et al.* 28, is an important open problem in the theory of ALFGs.

Another advantage of the ALFG is that one can implement these generators directly with floating-point numbers to avoid the constant conversion from integer to floating-point that accompanies the use of other generators. This is a distinct speed improvement when only floating-point numbers are required in the Monte Carlo computation. However, care must be taken to maintain the identity of the corresponding integer recursion when using the floating-point ALFG in parallel to maintain the uniqueness of the parallel streams. A discussion of how to ensure fidelity with the integer streams can be found in Brent 1.

ALFG, Marsaglia and Tsay 24, it has considered to be superior to ALFGs, parallel computing is ALFG

3 SPRNG

The SPRNG library is currently in it's first, full, Version 1.0 release. More-over SPRNG is now supported and maintained by NCSA under their high-performance software activities funded by the NSF under PACI. In addition, there has been considerable interest from most of the high-performance computing vendors in using SPRNG as a common, parallel pseudorandom number generation library on their machines. Thus SPRNG, itself, will be a lasting contribution to mathematical software for parallel Monte Carlo computations.

SPRNG is designed to use parameterized pseudorandom number generators to provide random number streams to parallel processes. SPRNG includes the following:

- Several, qualitatively distinct, well tested, scalable RNGs
- Initialization without interprocessor communication
- Reproducibility by using the parameters to index the streams
- Reproducibility controlled by a single "global" seed
- Minimization of interprocessor correlation with the included generators

- A uniform C, C++, FORTRAN, and MPI interface
- Extensibility
- An integrated test suite including physical tests

The decision to use parameterized generators was based on work of the author in parameterizing several different, common, RNGs to provide full-period streams of random numbers for each, unique, parameter value. These generators then formed the core of the generators currently available in SPRNG:

- Additive lagged-Fibonacci: $x_n = x_{n-r} + x_{n-s} \pmod{2^m}$
- Multiplicative lagged-Fibonacci: $x_n = x_{n-r} \times x_{n-s} \pmod{2^m}$
- Prime modulus multiplicative congruential: $x_n = ax_{n-1} \pmod{m}$
- Power-of-two modulus linear congruential: $x_n = ax_{n-1} + b \pmod{2^m}$
- Combined multiple recursive generator: $z_n = x_n + y_n \times 2^{32}$, where x_n is a linear congruential generator modulo 2^{64} and y_n satisfies $y_n = 107374182y_{n-1} + 104480y_{n-5} \pmod{2147483647}$

All the above generators can be thought of as being parameterized by a simple integer valued function, $f(\cdot)$ where $f(i)$ gives the appropriate parameter for the i th random number stream. Given this uniformity, the random number streams are mapped onto the binary tree through the canonical enumeration via the index i . This allows us to take the parameterization and use it to produce new streams from existing streams without the need for in-processor communication. We accomplish this by allowing a given stream access only to those streams associated with the subtree rooted at the given stream. This can be used to automatically manage static and dynamic creation of streams, and prohibits reuse of streams. To permit a calculation to be redone with different random numbers, we can apply a mixing function $p_s(\cdot)$ so that we map the streams onto the binary tree via the index $p_s(i)$ instead of just i . The function $p_s(\cdot)$ is a permutation parameterized by the global seed s . Different values of s give different permutations and thus map the streams onto the binary tree in different yet distinct ways.

SPRNG was also designed to be flexible, and to be as easy to use as possible. The Monte Carlo community is very conservative, and many groups use RNGs that have been handed down the generations (sometimes all the way back to Lehmer or Metropolis!). Thus we not only developed the library in collaboration with a member of this conservative community, but we

added the ability to extend the library with a user supplied generator. Thus a user may add their own RNG by rewriting two dummy SPRNG two routines and recompiling SPRNG. This then gives a user access to their own generator within the SPRNG parallel infrastructure. This is a powerful capability, and our own implementational experience has shown that any implementation must be thoroughly tested, empirically, to prevent unforeseen correlations within streams. (We found such unanticipated correlations ourselves in very carefully thought out implementations). Thus SPRNG includes a comprehensive testing suite to validate new generators. Together, the extensibility and testing suite aids both users wanting to implement their own generators in parallel, and provides library developers a powerful rapid prototyping tool.

Through the default generators, SPRNG is a tool for parallel pseudorandom number generation. The results obtained are also reproducible, and SPRNG provides a simple way to run on distributed-memory parallel machines using popular languages and parallel paradigms and supports distribution on a heterogeneous collection of machines.⁶ When a different RNG is desired, e.g. when a particular RNG is thought to give spurious results in a given application, a qualitatively different generator can replace the original by merely relinking the user program with SPRNG. Finally, new RNGs can be incorporated into SPRNG with little more than coding the generation and initialization routines and recompiling SPRNG.

4 Conclusions and Open Problems

We have presented a considerable amount of detail about parallel pseudorandom number generation through parameterization. In particular, we have described the SPRNG library as an example of a compressive library for parallel Monte Carlo.

While care has been taken in constructing generators for the SPRNG package, the designers realize that there is no such thing as a PRNG that behaves flawlessly for every application. This is even more true when one considers using scalable platforms for Monte Carlo. The underlying recursions that are used are for PRNGs are simple, and so they inevitably have regular structure. This deterministic regularity permits analysis of the sequences and is the PRNG's Achilles heel. Thus any large Monte Carlo calculation must be viewed with suspicion as an unfortunate interplay between the application and PRNG may result in spurious results. The only way to prevent this is

⁶In fact, the developers of CONDOR, a distributed computing tool, plan to incorporate SPRNG directly into CONDOR to make CONDOR a comprehensive tool for Monte Carlo on distributed heterogeneous collections of machines, see Litackow *et al.* ¹⁹

to treat each new Monte Carlo derived result as an experiment that must be controlled. The tools required to control problems with the PRNG include the ability to use another PRNG in the same calculation. In addition, one must be able to develop and use entirely new PRNGs as well. These capabilities as well as parallel and serial tests of randomness, Cuccaro *et al.*⁴, are components that make the SPRNG package unique among tools for parallel Monte Carlo.

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