LIFESPAN DISTRIBUTION OF SIMD GROUPS ON A GPU ENGAGED IN A CLASS OF PROBABILISTIC COMPUTATION

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ABSTRACT

In each SIMD (Single Instruction, Multiple Data) group, called a ‘warp’ of a GPU (Graphics Processing Unit), all the fixed number of threads execute the same instruction concurrently at each unit period of time. We consider a class of probabilistic algorithms designed for use on GPUs, including a wide variety of Monte Carlo methods, such that each thread contains a loop iterated stochastically variable times, and that the life-cycle of a warp ends when the slowest thread completes its requested task. A run-time model is proposed in order to explain the distributions of execution time observed in SIMD parallel computations using the algorithms of this class. Asymptotic properties of those distributions are also presented.

1. Introduction

Most of modern high-grade GPUs (Graphics Processing Units) have hundreds or thousands of cores (independent processing units) on their boards, which realize remarkably high performance in image processing by using SIMD (Single Instruction, Multiple Data) parallel technologies. Their use in a wide variety of computation other than 2D or 3D graphics, including weather dynamics and gas-liquid flow analysis, is known as GPGPU (General-Purpose use of GPU) and attracts attention of many workers engaged in various fields of science and technology (see, *e.g.*, Shimokawabe *et al.*, 2011).

In GPUs of SIMD architecture, each thread belongs to a SIMD group, comprised of a unit number (denoted by m , typically $m = 32$ or 64) of threads and called a ‘warp’ for those designed by nVIDIA, where a single common instruction is executed in each cycle of time (nVIDIA Corp., 2009). When a conditional branching happens, every thread in the warp may execute both *if-then* and *else* branches, but those threads which must not follow a given branch perform no-operations (denoted by **nops**) instead without any consequence. This probable inefficiency has induced workers to avoid implementing probabilistic algorithms on GPUs (Lee *et al.*, 2010, for instance), since they essentially involve many chances of conditional branching, despite the fact that GPGPU might be promising in a wide range of Monte Carlo computations.

On the other hand, in our preliminary experiments (Iida and Niki, 2013), we have observed that the more pseudo-random variates we generate by using rejection sampling in a thread on a GPU, the less run-time per variate we have. This fact stimulates us to design a run-time model discussed in this article for a particular class of probabilistic algorithms, including random walks and Monte Carlo methods with importance sampling, in each of

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which a block of instructions (called a ‘trial’ here) is repeated a randomly varying number of times.

The main target of this article is to give an approximation to the distribution of execution time observed in SIMD parallel configuration of a large number of cores. The results might be also useful in the design of GPGPU algorithms with stochastic behavior, because of the theoretically endorsed fact that well-organized and simplified probabilistic algorithms may be several tens of times or more, more efficient than those on a fast CPU in spite of existing negative reports.

2. Implementing Probabilistic Algorithms on GPU

2.1. A brief introduction to GPGPU

There are two principal merits in GPGPU. One is its superior parallel computing performance: a GPU consists of a great number of efficient cores designed for parallel performance, while a CPU consists of a few cores. Hardware implementation of elementary functions, *e.g.* logarithmic and trigonometric functions, in Super Function Units (SFUs) also attracts us especially in statistical computing. The other is its superb cost performance: GPUs are much cheaper than PC systems and can be equipped simply by inserting them in fast PCI Express buses built into almost all the latest motherboards for desktop PCs.

Two brands of GPUs are used worldwide, one is nVIDIA and the other is AMD (AMD, 2012). We focus only upon nVIDIA GPUs and use nVIDIA terminology, throughout this article, but the discussion here can also be applied to products by AMD and other vendors.

nVIDIA has been providing a program development environment called CUDA with which we can compose programs not only for multiple SIMD processes on a GPU, but also for bidirectional communication between CPU and GPU.

The GPU part of a job, called a ‘grid’, is started by a CPU request after its compiled codes have been sent through the fast PCI bus lines. A grid has exclusive use of a requisite number of GPU blocks called ‘streaming multiprocessors’, each of which provides computing resources, including cores, registers, function units, local and shared memories, to a ‘block’ of threads. If two or more blocks are allocated to a multiprocessor, they are consecutively processed.

Each ‘block’ consists of several ‘warps’, *i.e.*, SIMD groups of threads. The number of warps in a block is chosen to produce the optimum throughput depending the GPU architecture and the job. See ‘Cuda C programming guide’ (nVIDIA Corp., 2013) for more details.

2.2. Use of GPU in statistical computing including Monte Carlo calculation

It seems necessary to describe some details of the inefficiency commonly found in SIMD architecture mentioned in the introduction section.

Consider a simple case with two *if-then-else* blocks shown in Figure 1. If the logical variable P (*e.g.*, $P = (\text{PARAM} > 0)$) has the same value (**true** in this example) for all the m threads of a warp, then each thread executes only one branch (*i.e.*, B , the *if-then* branch). On the contrary, when there exist one **true** and one **false**, at least, among the truth values of Q (*e.g.*, $Q = (\text{rnd}() \leq 0.5)$) in the warp, then each thread executes both branches (in the optimal fixed order of execution; either D before E , or, E before D), provided that those threads which do not logically follow a given branch are flagged and make no effective action (shown as **nop**).

This architecture may involve severe inefficiency in speed, if the latter case with mixed

Fig. 1: SIMD operations in a warp with conditional branches.

truth values happens frequently, providing either D or E (or both) comprises a time consuming procedure. However, changing our viewpoints and considering the fact that no pipeline stall due to the branch takes place between B and F , we can rewrite the same preceding sentence as follows: “If both *if-then* and *else* branches consist of only a few operations, the overhead of conditional divergence is acceptable, even if the divergence quite frequently happens.”

The above circumstances appear in various kinds of statistical computations. The Metropolis method for numerical evaluation of the exact p -value for a given contingency table under the null hypothesis of independence, for example, involves full conditional transitions from a table to one of its neighboring tables. Monte Carlo composition of the sampling distribution of a statistic is another typical example, where a large number of samples from a population are generated for making a sequence of pseudo observations of a statistic. If rejection and/or composition techniques are applied in generation of random numbers distributed with a specified distribution one or more conditional branches take place for each random variate.

3. Run-time Model for SIMD Computation

3.1. Probabilistic algorithms with repetition of an identical procedure

We engage in discussions, in this article, on a class of probabilistic algorithms, including a wide variety of Monte Carlo methods. Each algorithm in this class consists a huge number of repeated execution of a probabilistic procedure which contains a stochastic number of trials. We first propose a run-time model for this class.

Consider a grid, the GPU part of a job, of which the goal is to obtain a huge number $k \times \ell$ of pseudo observations for a random variable. Parallel computation is performed by equally distributing the requisite procedures into ℓ threads. As shown in Figure 2, each thread belongs to a warp, the SIMD group, together with $m-1$ other threads and is required to obtain k independent observations.

If the number of trials varies for each observation, we need a special structure in designing the algorithm. For example, the flowchart (a) in Figure 3 is designed in order to follow the SIMD law in a faithful manner, where we can use a ‘vote’ family command for checking the allover status of threads in the warp. On the other hand, at the first glance, the

Fig. 2: Distributing procedures into threads of a grid

(a) satisfies SIMD law without effectual overhead.

(b) seems to violate SIMD law but works in some GPUs.

Fig. 3: SIMD flow of each thread in a warp.

trial	threads						
	0	1	2	3	4	...	$m-1$
1	—	○	○	—	○	...	—
2	○	○	—	○	○	...	○
3	—	●	○	○	—	...	○
4	—	●	●	—	●	...	●
5	○	●	●	●	●	...	●
6	●	●	●	●	●	...	●

○ : succeeded
 — : failed
 ● : done
 (3 successes)

Fig. 4: Example of probabilistic SIMD computation in a warp for $k = 3$.

flowchart (b) seems to violate the SIMD law, but works correctly on some (possibly many) GPUs. Here, synchronization can be done either explicitly by a system call in the program or implicitly by the warp management system.

Figure 4 shows an example of status changes in each thread of a warp during its lifespan. The fastest thread has completed its role at the third trial, in this example. In contrast, the most unlucky thread has needed 6 trials.

3.2. Distribution of the number of trials within a warp

For given positive integers m and k , let $(X_{nt})_{t \in \mathcal{K}}$ be a truncated recurrent renewal chain which represents how many trials have been done to obtain the t -th result in the n -th thread of a warp, where $\mathcal{K} = \{0, 1, \dots, k\}$ and $n \in \mathcal{M} = \{1, 2, \dots, m\}$. In the other words, the waiting times in $\{X_{nt} - X_{n,t-1} \mid n \in \mathcal{M}, t \in \mathcal{K} - \{0\}\}$ are *i.i.d.* positive integers, provided $X_{n0} = 0$ and $X_{nk} < \infty$, each of which signifies the number of trials until a success happens. Let Y and Z be the random variables

$$Y = \max_{n \in \mathcal{M}} X_{nk}, \quad Z = \min_{n \in \mathcal{M}} X_{nk}. \quad (1)$$

then the number of trials in a warp is given by Y as described in the previous subsection.

Let $F_k(x)$ and $f_k(x)$ be the cumulative distribution function (*cdf*) and the probability mass function (*pmf*) of X_{nk} , respectively, providing $F_k(x) = f_k(x) = 0$ for any $x \leq 0$. Then, the *cdf* $H_m^{(k)}(x)$ and the *pmf* $h_m^{(k)}(x)$ of Y are given as

$$H_m^{(k)}(x) = F_k(x)^m, \quad h_m^{(k)}(x) = F_k(x)^m - F_k(x-1)^m. \quad (2)$$

In any practical parallel algorithm, except experimental ones, we can assume the condition below:

Assumption 1 *All the moments of F_1 are finite.*

Either with or without Assumption 1, the following lemma is straightforward.

Lemma 1 *Let $\psi_k(s)$ and $\psi_1(s)$ be the characteristic functions for F_k and F_1 , respectively, then $\log \psi_k(s) = k \log \psi_1(s)$.*

From this lemma under Assumption 1, noting $\log \psi_1(s)$ and $\log \psi_k(s)$ are the cumulant generating functions, we have several corollaries.

Corollary 1 $\mathbb{E} X_{nk} = k\mu$ and $\text{Var} X_{nk} = k\sigma^2$, where $\mu = \mathbb{E} X_{n1}$ and $\sigma^2 = \text{Var} X_{n1}$.

Corollary 2 *The j -th cumulant κ_j^* for the standardized variable $(X_{nk} - k\mu)/\sqrt{k\sigma^2}$, satisfies the so-called Cornish-Fisher assumption, i.e., $\kappa_1^* \sim O(k^{-\frac{1}{2}})$ and $\kappa_j^* \sim O(k^{\frac{2-j}{2}})$ for $j \geq 2$.*

Corollary 3 X_{nk} has the limiting normal distribution $N(k\mu, k\sigma^2)$ as $k \rightarrow \infty$.

3.3. The repeat count k should be large enough

It might be most probable that one would implement the probabilistic algorithm shown in Figure 3 with $k = 1$ and repeat it k times considering the SIMD architecture of GPUs. In those cases, the number of trials Y' of each thread in a warp is given as

$$Y' = \sum_{i=1}^k \max_{n \in \mathcal{M}} X_{n1}^{(i)}, \quad X_{n1}^{(i)} \stackrel{i.i.d.}{\sim} F_1, \quad (3)$$

where **nops** are frequently executed in vain only to wait for the slowest thread in each iteration.

The expected value EY' is usually much larger than EY . For instance, consider the case that F_1 is the geometric distribution with probability parameter p , then

$$\begin{aligned} EY' &= k \sum_{x=1}^{\infty} x \left((1 - (1-p)^x)^m - (1 - (1-p)^{x-1})^m \right) \\ &\approx 3.428k \quad \left(\text{for } m = 32, p = \frac{3}{4} \right), \end{aligned} \quad (4)$$

On the other hand, by using the *cdf* of a negative binomial distribution,

$$\begin{aligned} EY &= \sum_{x=1}^{\infty} x \left(I_p(k, x-k+1)^m - I_p(k, x-k)^m \right) \\ &\approx \frac{4k\sqrt{k} + 5.984k + 4.845\sqrt{k} - 0.612}{3\sqrt{k} + 1.383} + \frac{0.283}{\sqrt{k+1} + 0.121} \\ &\quad \left(\text{for } m = 32, p = \frac{3}{4} \right), \end{aligned} \quad (5)$$

where $I_p(a, b)$ signifies the regularized incomplete beta function $B(p; a, b)/B(a, b)$. The above facts imply that a crude parallel algorithm corresponding to Y' will do, on average, more than 2 or 2.5 times more trials than the algorithm shown in Figure 3 for $k \geq 18$ or $k \geq 1,400$, respectively, in this example.

One may have noticed that the title of this subsection is demonstrated in (5) in an explicit form. Table 1 shows the expected numbers of trials for obtaining 10,000 results. From this table, it can be said that k should be tens or larger as far as total efficiency of computation attains its maximum with optimized resource allocation.

Table 1: Average numbers of trials for 10,000 results.

k	EY	$k'=10^4/k$	$k'EY$	
1	3.4279	10,000	34,279	
2	5.4000	5,000	27,000	
5	10.598	2,000	21,196	
10	18.577	1,000	18,577	
20	33.744	500	16,872	
50	77.354	200	15,471	
100	148.08	100	14,808	
500	698.48	20	13,970	
1,000	*1,377.9	10	*13,779	* extrapolated values by using (5).
10,000	*13,472	1	*13,472	

3.4. The limiting distribution of Y and its approximation

Hereafter, we discuss the cases where k is large enough (usually twenty or more under Assumption 1, say) to make the normal approximation in Corollary 3 practical. In the following discussions, Assumption 1 can be weakened as far as the central limit theorem holds for the distribution of X_{nk} for $k \rightarrow \infty$.

Let $\Phi(x)$ and $\phi(x)$ be the *cdf* and *pdf* of the standard normal distribution, respectively. Then, the limiting distribution of $(Y - k\mu)/\sqrt{k\sigma^2}$ for $k \rightarrow \infty$ has the *cdf* $H_m(x) = H_m^{(\infty)}(x) = \Phi(x)^m$ and the *pdf* $h_m(x) = m\phi(x)\Phi(x)^{m-1}$. See, *e.g.*, Gumbel (1947).

It is well known that H_m tends to a Gumbel distribution as $m \rightarrow \infty$, but the speed of convergence is too slow to use this fact for numerical computation in the typical cases, *i.e.*, $m = 32$ or 64 . Alternatively, we have found that H_{32} can be closely approximated by using a three parameter gamma distribution, $\text{Gamma}(13, \sqrt{\pi}/13, \sqrt{\pi}/6)$, where the parameters are chosen for mnemonic sake and can be replaced with optimal ones only a little superior in accuracy. Actually, for any $x \geq \sqrt{\pi}/6$,

$$\left| h_{32}(x) - \frac{13^{13}}{12! \pi^{13/2}} \left(x - \frac{\sqrt{\pi}}{6}\right)^{12} \exp\left(-\frac{13}{\sqrt{\pi}}\left(x - \frac{\sqrt{\pi}}{6}\right)\right) \right| < 0.02, \quad (6)$$

and the first six cumulants ν_j ($j = 1, \dots, 6$) of H_{32} are also approximated with differences less than 0.006:

$$\begin{aligned} \nu_1 - \frac{7\sqrt{\pi}}{6} &\approx 0.002, & \nu_2 - \frac{\pi}{13} &\approx -0.00004, & \nu_3 - \frac{2\pi^{3/2}}{13^2} &\approx -0.0002, \\ \nu_4 - \frac{3!\pi^2}{13^3} &\approx 0.006, & \nu_5 - \frac{4!\pi^{5/2}}{13^4} &\approx 0.004, & \nu_6 - \frac{5!\pi^3}{13^5} &\approx -0.0006. \end{aligned} \quad (7)$$

Similar approximation can be also applicable to H_m for a wide range of m .

3.5. Distribution of run-time for a trial

Let R_j denote the run-time of the j -th trial, which is common to every thread of a warp because of SIMD operation. In the probabilistic algorithms concerned, R_j can be considered as a discrete random variable distributed with a distribution G_c , where c is the number of active threads in the warp at the j -th trial, *i.e.*,

$$c = c(j) = \#\{n \in \mathcal{M} \mid X_{nk} \geq j\}. \quad (8)$$

Unless the programming code contains some kind of bug, it can be said, as seen in Figure 5, that

1. The support of G_c comprises several fixed points of time corresponding to all the possible paths through the conditional branches in a trial and to all the possible delays caused by memory access fluctuations.
2. G_c is almost a one point distribution when c is large enough, like G_{32} in Figure 5.
3. As c decreases from m to 1, the possibility of taking the slowest path through all the *if-then* and *else* blocks becomes smaller.
4. As a result of the above, the expectation of R_j decreases as j increases beyond Z .

Fig. 5: An example of $\{G_m, \dots, G_1\}$ ($m = 32$) with a single conditional branch.

From these, the following assumption is posited hereafter.

Assumption 2 For any $c \in \mathcal{M}$, the support of G_c is included within a fixed interval $[a, b]$ and, as a consequence, all the r -th cumulants ρ_{cr} ($r = 1, 2, \dots$) of G_c are finite; providing the sequence of means is descending as c runs from m to 1, i.e.,

$$\rho_{m1} \geq \rho_{(m-1)1} \geq \dots \geq \rho_{21} \geq \rho_{11}. \quad (9)$$

The relative relations in (9) would hold for carefully designed algorithms. Even if some inequalities may not hold, there exists a clearly declining tendency.

4. Approximation for Lifespan Distribution of a Warp

4.1. Lifespan time L_Y of a warp

Providing a random variable R_0 with finite cumulants to represent the total time spent for preceding and succeeding operations to the part of iterating trials, we can write the lifetime L_Y of a warp as

$$L_Y = \sum_{j=0}^Y R_j = L_Z + \sum_{j=Z+1}^Y R_j, \quad L_Z = R_0 + \sum_{j=1}^Z R_j. \quad (10)$$

where each of $\{R_j \mid j = 1, \dots, Z\}$ is independently distributed with G_m .

Concerning the distributions of L_Y , the following lemma plays an essential role.

Lemma 2 As $k \rightarrow \infty$, $Y/k \xrightarrow{P} \mu$ and $(Y - Z)/k \xrightarrow{P} 0$.

Proof. From Corollary 1, for any $d > 0$, the Chebyshev inequality gives

$$\begin{aligned} \Pr\{Y - k\mu \geq d\} &= \Pr\{(X_{1k} - k\mu \geq d) \vee \dots \vee (X_{mk} - k\mu \geq d)\} \\ &\leq \Pr\{X_{1k} - k\mu \geq d\} + \dots + \Pr\{X_{mk} - k\mu \geq d\} \\ &\leq m \Pr\{|X_{1k} - k\mu| \geq d\} \leq \frac{mk\sigma^2}{d^2}, \end{aligned} \quad (11)$$

and, in similar manner,

$$\Pr\{k\mu - Z \geq d\} \leq \frac{mk\sigma^2}{d^2}. \quad (12)$$

Hence, for any $\varepsilon > 0$, $\delta > 0$ and $k > \frac{8m\sigma^2}{\delta\varepsilon^2}$, it holds that

$$\begin{aligned} \Pr\left\{\frac{Y-Z}{k} > \varepsilon\right\} &= \Pr\{(Y - k\mu) + (k\mu - Z) > \varepsilon k\} \\ &\leq \Pr\left\{(Y - k\mu > \frac{\varepsilon k}{2}) \vee (k\mu - Z > \frac{\varepsilon k}{2})\right\} \\ &\leq \Pr\{Y - k\mu > \frac{\varepsilon k}{2}\} + \Pr\{k\mu - Z > \frac{\varepsilon k}{2}\} \leq \frac{8m\sigma^2}{k\varepsilon^2} < \delta. \end{aligned} \quad (13)$$

and also

$$\begin{aligned} \Pr\left\{\left|\frac{Y}{k} - \mu\right| > \varepsilon\right\} &= \Pr\{Y - k\mu > \varepsilon k\} + \Pr\{k\mu - Y > \varepsilon k\} \\ &\leq \Pr\{Y - k\mu > \varepsilon k\} + \Pr\{k\mu - Z > \varepsilon k\} \leq \frac{2m\sigma^2}{k\varepsilon^2} < \delta. \end{aligned} \quad (14)$$

Lemma 3 Assume that R_0 has a finite upper bound, then, as $k \rightarrow \infty$,

$$\frac{L_Y}{k} \xrightarrow{P} \frac{L'_Y}{k} = \frac{1}{k} \sum_{j=1}^Y R'_j, \quad R'_j \stackrel{i.i.d.}{\sim} G_m.$$

Proof. For $1 \leq j \leq Z$, noting $R_j \stackrel{i.i.d.}{\sim} G_m$, we can replace R'_j with R_j . Hence, by noting Assumption 2, Lemma 2 gives

$$\begin{aligned} \left|\frac{L_Y - L'_Y}{k}\right| &\leq \frac{1}{k} \left(R_0 + \sum_{j=Z+1}^Y |R_j - R'_j|\right) \\ &\leq \frac{\bar{R}}{k} + \frac{Y-Z}{k} (b-a) \xrightarrow{P} 0 \quad (k \rightarrow \infty), \end{aligned} \quad (15)$$

where $\bar{R}$ is the upper bound of R_0 . ■

Usually, the difference $|R_j - R'_j|$ in (15) is small even in the case that $R_j \sim G_1$. Then, L'_Y gives an approximation to L_Y precise enough to use in practical applications.

4.2. The limiting distribution of L'_Y/k

The cumulants of the limiting distribution of L'_Y/k as $k \rightarrow \infty$ are directly obtained from Lemmas 1 and 3 of this article and Theorem 1 in Niki *et al.* (1990).

Theorem 1 Let ν_s and ρ_s denote the s -th cumulant of H_m and G_m . Then, the s -th cumulant λ_s of the limiting distribution of L'_Y/k is given as

$$\lambda_s = \sum_{\pi(s)} \frac{s!}{r_1! r_2! \cdots r_s! (1!)^{r_1} (2!)^{r_2} \cdots (s!)^{r_s}} \nu_q \rho_1^{r_1} \rho_2^{r_2} \cdots \rho_s^{r_s}, \quad (16)$$

where the summation goes over all partitions $\pi(s)$ of s , i.e.,

$$\pi(s) = \{(1^{r_1} 2^{r_2} \cdots s^{r_s}) \mid (r_1, r_2, \dots, r_s) \in \mathbb{N}^s, r_1 + 2r_2 + \cdots + sr_s = s\}$$

with $q = r_1 + r_2 + \cdots + r_s$.

Corollary 4 *The first four cumulants are given as follows:*

$$\begin{aligned} \lambda_1 &= \nu_1 \rho_1, & \lambda_2 &= \nu_2 \rho_1^2 + \nu_1 \rho_2, & \lambda_3 &= \nu_3 \rho_1^3 + 3\nu_2 \rho_1 \rho_2 + \nu_1 \rho_3, \\ \lambda_4 &= \nu_4 \rho_1^4 + 6\nu_3 \rho_1^2 \rho_2 + \nu_2(4\rho_1 \rho_3 + 3\rho_2^2) + \nu_1 \rho_4. \end{aligned} \quad (17)$$

Corollary 5 *If G_m can be approximated with a one point distribution, like G_{32} in Figure 5, then, since $\rho_j \approx 0$ ($j \geq 2$),*

$$\lambda_1 \approx \nu_1 \rho_1, \quad \lambda_2 \approx \nu_2 \rho_1^2, \quad \lambda_3 \approx \nu_3 \rho_1^3, \quad \lambda_4 \approx \nu_4 \rho_1^4, \quad \dots, \quad (18)$$

which mean that L'_Y/k can be approximated with a gamma distribution.

Remark 1 Similar discussion gives that the distribution of L_Z/k can be approximated with a ‘reversed’ gamma distribution of which the *pdf* is the reflected image of a ‘usual’ gamma density. Correctness of approximation would be more precise than that for L_Y/k .

Remark 2 From the inequalities in (9), there exists a clear tendency that, for the larger value of Y , the difference $R'_j - R_j$ has the larger expected value. This fact implies that the scale and location parameters of the best-fit gamma distribution for L_Y/k are a little smaller than those for L'_Y/k . On the other hand, the shape parameter for L_Y/k is larger than that for L'_Y/k because of smaller skewness.

5. Monte Carlo Computation with Envelope Rejection — an Example

5.1. Random number generation with envelope rejection

Consider a weighted Monte Carlo integration of a designated function $w(x)$, *i.e.*,

$$\int_{-\infty}^{\infty} w(x)v(x) dx \approx \frac{1}{N} \sum_{j=1}^N w(V_j) \quad (19)$$

where $V_1, \dots, V_N$ are random variates independently distributed with a *pdf* $v(x)$. It is well known that the accuracy of approximation is proportional to $1/\sqrt{N}$.

Envelope rejection is one of the most popular techniques for generating a random variate $V \sim v(x)$ and is applicable if there exists a *pdf* $q(x)$ such that $(\forall x, 0 < \exists p < 1) pv(x) \leq q(x)$ and the random variate $Q \sim q(x)$ is generated fast. An outline of the generation procedure can be written as follows:

1. Generate a pair of random variates (Q, U) where $U \sim \text{Uniform}[0, 1]$.
2. If $Uq(x) \leq pv(x)$ accept Q as V , otherwise go back to (1).

The probability of acceptance is p .

When we use $\ell = N/k$ threads, *i.e.*, $\ell/m = N/(km)$ warps on a GPU for this numerical integration, the number X of trials made in a thread for generating k random variates has the negative binomial distribution with the *pmf*

$$f_k(x) = \binom{x-1}{k-1} p^k (1-p)^{x-k} \quad (x \geq k) \quad (20)$$

of which first four cumulants are given, reflecting Lemma 1, as

$$\kappa_1 = \frac{k}{p}, \quad \kappa_2 = \frac{k(1-p)}{p^2}, \quad \kappa_3 = \frac{k(1-p)(2-p)}{p^3}, \quad \kappa_4 = \frac{k(1-p)(p^2 - 6p + 6)}{p^4}. \quad (21)$$

For numerical illustration, the method due to Ahrens and Dieter (1974) is used here for generating gamma variates with shape parameter $1/2$, *i.e.*,

$$v(x) = \frac{1}{\sqrt{\pi}} x^{-\frac{1}{2}} e^{-x}, \quad q(x) = \begin{cases} \frac{p}{\sqrt{\pi}} x^{-\frac{1}{2}} & \text{for } x \leq 1 \text{ with probability } p_0, \\ \frac{p}{\sqrt{\pi}} e^{-x} & \text{for } x > 1 \text{ with probability } 1 - p_0, \end{cases} \quad (22)$$

where

$$\mu = \frac{1}{p} = \frac{e\sqrt{\pi}}{1+2e} \approx 1.336, \quad p_0 = \text{erf}(1) \approx 0.843. \quad (23)$$

Then, a trial has three conditional branches with $3^3 = 27$ possible execution paths, which makes the difference $|R'_j - R_j|$ ($j > Z$) not negligible.

5.2. Gamma distributions fitted to empirical lifespan distributions

An empirical distribution of L_Y/k observed in the Monte Carlo integration of $w(x) = x^2$ with $V \sim v(x)$ in (22) is shown as the histogram with gray bars in Figure 6. The integration has been done on an nVIDIA Tesla C2070 with 448 cores and clock rate of 1.147 GHz, by letting $N = 448 \times 1,000$ and $k = 1,000$. The solid line represents the *pdf* of the fitted gamma distribution $\text{Gamma}(21, 0.00893, 6.915)$ to the observations.

The dashed line represents the imaginary distribution of L'_Y/k drawn as the *pdf* of $\text{Gamma}(13, 0.01363, 6.939)$. These parameters are brought from the best-fit distribution $\text{ReversedGamma}(13, 0.01363, 6.880)$ to the empirical distribution of L_Z/k , which is expressed as the histogram with white bars. As stated in Remark 1, the location parameter is given by using $6.939 \approx 6.880 + 2 \times 0.01363 \times 13/6$. In addition, as noted in Remark 2, the distribution of L_Y/k has a larger shape parameter and smaller scale and location parameters than those for L'_Y/k , correspondingly.

All the CUDA codes in C++, both those run on GPU and on CPU together, are compiled and executed through CUDA Link, the CUDA interface built in Mathematica (see Wolfram Research Inc., 2013, for details).

Fig. 6: Lifespan distribution of warps in gamma random number generation

6. Concluding Remarks

Not only in Monte Carlo integration but in various kinds of statistical GPGPU experiments, we have observed the similar gamma-distribution-shaped distributions. Sometimes approximation by using L'_Y happens to give a quite close estimate to the target, and some other times it furnishes just a rough sketch of the actual observations as seen in the example in Section 5.

For most readers, the important thing may not be just how accurate the approximation is, but how instrumental the results given here are for designing statistical GPGPU algorithms. From this viewpoint, we might have already confirmed the following two assertions:

1. Statistical GPGPU could be efficient by employing properly designed algorithms, at least for purposes of a particular kind.
2. Allocation size k to each thread should be large enough with due consideration of resource allotment.

For designing practical GPU algorithms of higher performance, we need additional well-established techniques, of course, including memory resource management and memory latency hiding.

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REFERENCES

- Advanced Micro Devices (AMD), Inc. (2012), *Getting Started with SequenceL — Optimizing Parallel Processing Performance and Coding Efficiency with AMD APUs and Texas Multicore Technologies' SequenceL Auto-parallelizing Programming Solution*, AMD White Paper, AMD Incorporated.
- Ahrens, J. H. and Dieter, U. (1974), Computer methods for sampling from gamma, beta, Poisson and binomial distributions, *Computing*, **12**, 223–246.
- Gumbel, E. J. (1947), The distribution of the range, *Annals of Mathematical Statistics*, **18**(3), 384–412.
- Iida, M. and Niki, N. (2013), GPGPU for probabilistic algorithms with heavily repeated identical procedures (in Japanese), *Proceedings of the 27th Symposium of Japanese Society of Computational Statistics*, 35–36.
- Lee, A., Yau, C., Giles, M. B., Doucet, A. and Holmes, C. C. (2010), On the utility of graphics cards to perform massively parallel simulation of advanced Monte Carlo methods, *Journal of Computational Graphics and Statistics*, **19**(4), 769–789.
- Niki, N., Nakagawa, S. and Inoue, H. (1990), Cumulants of random sum distributions, *Communication in Statistics – Theory and Methods*, **19**(5), 1857–1861.
- nVIDIA Corp. (2009), *nVIDIA's Next Generation CUDA: Fermi*, White Paper, nVIDIA Corporation.
- nVIDIA Corp. (2013), *Cuda C Programming Guide*, nVIDIA Corporation.

Shimokawabe, T., Aoki, T., Ishida, J., Kawano, K. and Muroi, C. (2011), 145 TFlops performance on 3990 GPUs of TSUBAME 2.0 supercomputer for an operational weather prediction, *Procedia Computer Science*, **4**, 1535–1544.

Wolfram Research Inc. (2013), *CUDALink*,

<http://reference.wolfram.com/mathematica/CUDALink/guide/CUDALink.html>

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