Monte Carlo integration on GPU

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Abstract. We use a graphics processing unit (GPU) for fast computations of Monte Carlo integrations. Two widely used Monte Carlo integration programs, VEGAS and BASES, are parallelized on GPU. By using $W^+\text{ plus multi-gluon}$ production processes at LHC, we test integrated cross sections and execution time for programs in FORTRAN and C on CPU and those on GPU. Integrated results agree with each other within statistical errors. Execution time of programs on GPU run about 50 times faster than those in C, and more than 60 times faster than the original FORTRAN programs.

1 Introduction

GPU (Graphics Processing Unit) is originally developed for fast output of moving complex images onto computer displays. Because it is composed of many multi-processors, it can be used as a powerful parallel processor not only for graphics applications but also for general purpose computations. GPU has already been used in scientific applications which require a huge number of calculations to process data as in astrophysics and fluid dynamics. Also in elementary particle physics, successful computations of various cross sections on GPU have been reported in [1, 2]. In these studies programs on GPU were shown to run about 100 times faster than those on CPU.

Two-orders of magnitude reduction of computation time by GPU demonstrated in the previous studies should greatly improve the efficiency of analysis in the field of elementary particle physics. In this paper, we show that general purpose Monte Carlo integration programs can be adopted to run on GPU, opening the door of fast and economical computation to all area of research that makes use of Monte Carlo method.

2 Monte Carlo integration programs

Scattering amplitudes of physics processes at LHC energies are expressed as complex functions of momenta and helicities of external particles, and kinematical distributions of produced particles are obtained by integrals of the squared amplitudes over many-body phase space. Because integration of multi-dimensional function is most conveniently done with Monte Carlo integration technique, the method is widely used in the field of elementary particle physics. They are especially useful when evaluating differential cross sections with experimental cuts on produced particle momenta.

As the number of final state particles increases, the computation time which is necessary to obtain good accuracy of the integrated results grows quickly. It is partly because the number of sampling points during the integration should be higher for higher dimensional integral, and partly because the computation time for the scattering amplitudes also increases as the number of external particles grows. Therefore, integration of differential cross section with good accuracy becomes a very time consuming task for multi-particle productions processes. Significant reduction of computation time by the use of GPU will contribute to the improvement of the efficiency of physics analysis at LHC and elsewhere.

VEGAS [3] and its variants are widely used for Monte Carlo integration. They are based on an iterative and adaptive Monte Carlo scheme. In these programs each axis of variable is divided into grids, thus the integrand volume is divided into hypercubes. Monte Carlo integration is performed in each hypercube and variances from hypercubes are used to define new grid spacings which are used in the next iteration step. The variance of total integral is reduced by iteration by iteration. BASES [4] is one of its variants developed at KEK, which has been widely used in particle physics at colliders.

In this paper we study parallelization of VEGAS and BASES, by using GPU.

3 Parallelization of Monte Carlo integration program

3.1 Program structure

Multi-dimensional integration programs, VEGAS and BASES, have the following common structure:

1. initialize parameters,
2. generate a space point within a $k$-dimensional hypercube from a set of $k$ random numbers,
3. compute an integrand function at the generated space point,
4. accumulate function values,
5. optimize grid spacing after accumulating $N$ function values,
6. repeat 2-5 steps up to $M$ iterations or until the desired accuracy is reached.

In BASES, after $M$ iterations (grid optimization phase) are done, further iteration steps are executed in order to improve the accuracy of the integration (integration phase). The results of this integration phase are used for event generations by SPRING [4].

We measure fractions of CPU time for each step and find that almost 98-99% of total CPU time is used in the step 3 where integrand function is computed. This fraction grows as the number of sampling points grows and the complexity of the integrand function grows. Therefore significant reduction of total CPU time is expected by parallelizing function calls at all sampling points with GPU.

### 3.2 Program conversion

Both VEGAS and BASES are originally written in FORTRAN. In order to transfer function calls to GPU, they should be written in CUDA [5], C/C++ style platform developed for general purpose computing on GPU. We first convert the FORTRAN programs into C codes. Then we transform the function call part further into CUDA codes. Due to the limited support for double precision computation capabilities of the GPU which we use for this study [4], floating point computations in the GPU programs are done in single precision [5].

In the programs of GPU version, all sampling points are generated on GPU and integrand function values at each space point is computed in parallel (steps 2-3). Then computed function values are transferred to CPU memories. At the CPU side, computed function values are accumulated and grid parameters are optimized based on the accumulated information (steps 4-5). These steps are iterated and variance of integral are reduced.

### 4 Computing environments

#### 4.1 GPU and its host PC

We use a GeForce GTX285 by NVIDIA [7] for the computation of cross sections of physics processes with Monte Carlo integration. The GeForce GTX285 which is connected with PCI Express x16 bus has 30 streaming multiprocessors (SM). Since each SM has 8 streaming processors (SP), the GTX285 GPU card has 240 SP in total.

Other parameters of the GTX285 are summarized in Table 1. The GTX285 is controlled by Linux PC with Fedora10 (64bit) operating system. The parameters of host computer is summarized in Table 2.

In order to compile programs of GPU version, we use the CUDA version 2.3 toolkit which are obtained from the NVIDIA site [4]. And for the programs in FORTRAN and C, we use gfortran and gcc which is automatically installed with Fedora 10. The version of compilers are summarized in Table 3.

| Number of multiprocessor | 30 |
|--------------------------|----|
| Number of core           | 240|
| Total amount of global memory | 2GB |
| Total amount of constant memory | 64kB |
| Total amount of shared memory per block | 16kB |
| Total number of registers available per bloc | 16kB |
| Clock rate               | 1.48GHz |

| CPU                      | Core i7 2.67GHz |
|--------------------------|----------------|
| L2 Cache                 | 8MB            |
| Memory                   | 6GB            |
| Bus Speed                | 1.333GHz       |
| OS                       | Fedora 10 (64 bit) |

| nvcc                     | Rel. 2.3 (V0.2.1221) |
|--------------------------|----------------------|
| CUDA Driver              | Ver.2.30             |
| CUDA Runtime             | Ver 2.30             |
| gfortran                 | 4.3.2 (Red Hat 4.3.2-7) |
| gcc                      | 4.3.2 (Red Hat 4.3.2-7) |

#### 4.2 Process time measurement

For process time measurement, we measure the time between the start of VEGAS/BASES programs and the completion of them, i.e. between the step 1 and the completion of the step 6, including the steps 4 and 5 that are processed on CPU. For FORTRAN programs, an intrinsic procedure of gfortran, “cpu.time”, is used for the measurement of elapsed CPU time. For C and GPU programs, a system call, “getrusage”, is used for the time measurements.
5 Physics process

In order to test the GPU version of VEGAS and BASES, called gVEGAS and gBASES respectively, we compare total cross sections of multi-particle production process at LHC. In particular, we report results on the following processes

\[
\bar{u}d \rightarrow W^+ (\rightarrow \mu^+ \nu_\mu) + n \text{ gluons } (n = 0 \sim 4) \tag{1}
\]

with semi-realistic final state cuts at LHC. The dimension of integral is \(3(n+2)-4\) from the phase space, 2 from the parton distributions (PDF), and 1 for the helicity summation, and hence \(3n+5\); hence from 5-dimensional integral for no gluon \((n = 0)\) to 17-dimensional integral for 4 gluons \((n = 4)\).

The degree of the complexity (length) of the integral function can be estimated from the number of contributing Feynman diagrams and the number of independent color-basis vectors as listed in Table 4. Previous studies \([1]\) show that the performance of GPU computation is limited by the product of these two numbers, the processes eq. (1) cover program size of four orders of magnitude difference.

In order to simulate realistic LHC experiments, we introduce the following final state cuts. For gluons,

\[
|\eta| < 5, \quad p_{T_i} > 20 \text{ GeV}, \quad p_{T_{ij}} > 20 \text{ GeV}, \tag{2}
\]

where \(\eta\) and \(p_{T_i}\) are the rapidity and the transverse momentum of the \(i\)-th jet, respectively, in the \(pp\) collisions rest frame along the right-moving \((p_\mu = |p|)\) proton momentum direction, and \(p_{T_{ij}}\) is the relative transverse momentum \([8]\) between the jets \(i\) and \(j\) defined by

\[
p_{T_{ij}} \equiv \min(p_{T_i}, p_{T_j}) \Delta R_{ij}, \tag{3a}
\]

\[
\Delta R_{ij} = \sqrt{\Delta \eta_{ij}^2 + \Delta \phi_{ij}^2}. \tag{3b}
\]

Here \(\Delta R_{ij}\) measures the boost-invariant angular separation between jets. For \(\mu^+\) from \(W^+\) decay, we require

\[
|\eta| < 2.5, \quad p_{T} > 20 \text{ GeV} \tag{4}
\]

As for the parton distribution function (PDF), we use the set CTEQ6L1 \([9]\) and the factorization scale is chosen to be the \(Z\) boson mass. The QCD coupling constant is also fixed as \(\alpha_s(m_Z)_{CTEQ6L1} = 0.118\) \([10]\).

For the computation of helicity amplitudes of these processes, HELAS \([11]\) for FORTRAN programs and its C/GPU version, HEGET \([12]\) are used.

| Table 4. \(\bar{u}d \rightarrow W^+ (\rightarrow \mu^+ \nu_\mu) + \text{gluons}\) |
|-----------------|-----------------|-----------------|
| Number of gluons | Number of diagrams | Number of color bases |
| 0               | 1               | 1               |
| 1               | 2               | 1               |
| 2               | 8               | 2               |
| 3               | 54              | 6               |
| 4               | 516             | 24              |

| Table 5. Parameters for integrations |
|-----------------|-----------------|-----------------|-----------------|
| Number of gluons | NCALL | ITMX | ITMX1 | ITMX2 |
| 0               | \(10^6\) | 10   | 5     | 5     |
| 1               | \(10^6\) | 10   | 5     | 5     |
| 2               | \(10^6\) | 10   | 5     | 5     |
| 3               | \(10^7\) | 10   | 5     | 5     |
| 4               | \(10^7\) | 10   | 5     | 5     |

6 Results

6.1 Parameters of the integration programs

In order to control the behavior of the Monte Carlo integration by VEGAS and BASES, user can give them the following parameters:

- number of total function calls in one iteration step \((\text{NCALL})\),
- number of maximum iteration steps \((\text{ITMX})\), and
- desired accuracy of the integration \((\text{ACC})\).

\text{NCALL} is the number \(N\) in step 5 and \text{ITMX} is the number \(M\) of the step 6 in Section 5.1. Iteration steps of BASES are separated into two phases: the grid optimization step and the integration step. Accordingly, \text{ITMX} and \text{ACC} are also separated as:

- number of maximum iteration steps \((\text{ITMX1})\), and
- desired accuracy of integration \((\text{ACC1})\)

for the grid optimization phase, and

- number of maximum iteration steps \((\text{ITMX2})\), and
- desired accuracy of integration \((\text{ACC2})\)

for the integration phase.

Parameter values used in this study are summarized in Table 5. In order to keep the total amount of computations to be the same among all the programs, all desired accuracies, \text{ACC} for VEGAS and \text{ACC1} and \text{ACC2}, are set to an extremely small value \((0.001\%)\) which cannot be reached by MC sampling of \text{NCALLxITMX} points used in this study: see Table 5. For BASES, numbers of iteration steps for the grid optimization and integration phases are set to be equal \((\text{ITMX1} = \text{ITMX2})\), and their sum is set the same as \text{ITMX} of VEGAS programs \((\text{ITMX1}+\text{ITMX2} = \text{ITMX})\). In summary, we accumulate \(10^7\) sample points for processes up to two gluons \((n = 0, 1, 2)\) and \(10^8\) points for those with more gluons \((n = 3 \text{ and } 4)\).
6.2 Total cross section computation

Total cross sections for processes in eq. (11) with experimental cuts (eqs. [24]) are listed in Table 6. They are computed with programs in FORTRAN, C and CUDA (GPU). Cross sections from different of programs agree to each other within their statistical errors. In addition, they agree with the results from the event generator MadGraph/MadEvent [12][13][14].

6.3 Parameters of the kernel program

The performance of GPU programs largely depends on parameters of kernel programs executed on GPU. Most significant parameters which affect the process time of programs are:
- number of registers allocated to a thread, and
- number of threads in a thread block.

Details of kernel parameters are explained in [1]. In this study we use 64 as a number of registers allocated a thread and 256 as a number of threads in a thread block. From the detailed study of dependence of performance on these parameters we find that they give almost the best performance for all processes in this study.

Number of thread blocks in a grid (= a set of thread blocks), which is executed with a single kernel call, are set to be equal to NCALL, so that one iteration of Monte Carlo integration steps is executed by a single kernel call.

6.4 Process time comparisons

In Table 7, measured process time for a single function call is listed for all programs. As explained above, the process time per single function call is obtained by dividing the total computation time by $10^7$ for processes with up to two gluons ($n = 0, 1, 2$) and by $10^8$ for those with more gluons ($n = 3$ and 4).

Numbers in parentheses in the FORTRAN and C columns in Table 7 are the ratio of the process time as compared to that of GPU. About a factor of 50 times more sampling is possible with GPU as compared to the C programs on CPU. During the comparison of process time, we find that the original FORTRAN codes run slower than the C-version. Because the total process time for these CPU programs is dominated by the function (amplitude) computation, this FORTRAN-to-C ratio can be originated from the difference of handling complex numbers which appears in amplitude computations. We use in-line functions for the computations of complex numbers in C, which might have better efficiency compared with built-in complex functions in FORTRAN.

In Fig. 1 process time for a single function call is plotted against the number of gluons in the final state. And in Fig. 2 ratios of process time between programs on CPU (FORTRAN/C) and those on GPU are plotted. Differences of process time between VEGAS and BASES are small. Programs which are executed on GPU can run about 50 times faster than those in C. Compared with original FORTRAN version programs, the differences of performance become larger.

When the final state has 4 gluons, the size of GPU program becomes large and requires more access to local memories. From previous studies on performances of GPU programs [11], larger programs show worse performance on execution time. Still the VEGAS(BASES) programs for the 4 gluon production process runs 40 (34) times faster on GPU than the C-program runs on CPU.

| No. of gluons | FORTRAN | VEGAS | BASES | FORTRAN | C | GPU | FORTRAN | C | GPU | MG/ME | [fb] |
|--------------|---------|-------|-------|---------|---|-----|---------|---|-----|-------|-----|
| 0            | 2.137±0.001 | 2.137±0.001 | 2.137±0.001 | 2.137±0.001 | 2.137±0.001 | 2.137±0.001 | 2.137±0.001 | 2.137±0.001 | 2.138±0.002 | $10^6$ |
| 1            | 1.783±0.001 | 1.783±0.001 | 1.780±0.001 | 1.785±0.001 | 1.784±0.001 | 1.782±0.001 | 1.773±0.003 | $10^5$ |
| 2            | 1.873±0.007 | 1.853±0.006 | 1.843±0.006 | 1.876±0.007 | 1.863±0.010 | 1.870±0.007 | 1.874±0.002 | $10^4$ |
| 3            | 2.868±0.008 | 2.881±0.009 | 2.832±0.010 | 2.860±0.010 | 2.855±0.014 | 2.907±0.012 | 2.845±0.005 | $10^3$ |
| 4            | 6.186±0.041 | 6.054±0.081 | 6.157±0.073 | 6.078±0.134 | 6.191±0.068 | 6.385±0.235 | 6.070±0.010 | $10^2$ |

Table 6. Total cross sections of $u\bar{d} \rightarrow W^+ (\rightarrow \mu^+ \nu_\mu) + n$-gluons computed by programs in FORTRAN, C, CUDA (GPU) and MadGraph/MadEvent.
Table 7. Process time for a single function call in VEGAS and BASES on CPU with FORTRAN or C, and on GPU with CUDA. Numbers in the parentheses of the FORTRAN and C columns are the ratio of process time relative to that of GPU.

| No. of gluons | VEGAS [μsec] | BASES [μsec] |
|---------------|--------------|--------------|
|               | FORTRAN | C | GPU | FORTRAN | C | GPU |
| 0             | 1.32 (63.8) | 1.06 (51.2) | 0.0207 | 1.78 (68.7) | 1.39 (53.5) | 0.0260 |
| 1             | 2.19 (68.8) | 1.73 (54.6) | 0.0318 | 2.97 (75.0) | 2.24 (56.6) | 0.0396 |
| 2             | 4.19 (84.2) | 2.96 (59.5) | 0.0497 | 4.97 (88.3) | 3.35 (59.6) | 0.0563 |
| 3             | 11.1 (101)  | 7.00 (63.6) | 0.110 | 11.7 (103)  | 7.02 (62.2) | 0.113 |
| 4             | 72.1 (77.8) | 37.4 (40.4) | 0.927 | 61.6 (66.2) | 31.8 (34.2) | 0.931 |

Fig. 2. Process time ratios of FORTRAN and C programs to the corresponding GPU program.

7 Summary

Based on VEGAS and BASES programs written in FORTRAN, we have developed Monte Carlo integration programs, gVEGAS and gBASES respectively, which can be executed on NVIDIA’s GPU using the CUDA development kit. We have tested their performance with the computation of total cross sections of processes, \( u\bar{d} \rightarrow W^+ \rightarrow \mu^+\nu_\mu \) + n-gluons \((n = 0 \sim 4)\), in \( pp \) collisions at \( \sqrt{s} = 14\text{TeV} \). Total cross sections agree with each other within statistical errors for all programs. Both VEGAS and BASES programs on GPU run about 50 times faster than the same programs written in C, which are converted from the original FORTRAN version programs. Compared with FORTRAN programs their GPU version programs show more than 60 times better performance in execution time. For the process with 4 gluons, the size of GPU programs becomes large and their relative performance become worse than small programs.

Appendix A Sample codes for gVEGAS

Sample source codes of the gVEGAS program are available from the web page: http://madgraph.kek.jp/KEK/GPU/gVEGAS/example/. They include a minimum set of source files which are necessary to do Monte Carlo integration with the VEGAS algorithm on GPU, but do not include Makefile which largely depends on user’s environment of development.

Appendix A.1 User programs

Sample codes include two user programs: gVegasMain.cu and gVegasFunc. They should be customized by user to the task one intends to perform.

Appendix A.1.1 gVegasMain.cu

gVegasMain.cu includes a sample main program for Monte Carlo integration where user can set parameters for the integration. Typical parameters are:

- \( n\text{BlockSize} \): size of a thread block of a kernel program on GPU
- \( \text{ndim} \): number of independent variables of integrand function
- \( \text{ncall} \): number of sample points per iteration
- \( \text{itmx} \): maximum number of iterations
- \( \text{acc} \): required accuracy during iterations

All these parameters can be set within gVegasMain.cu.

Appendix A.1.2 gVegasFunc.cu

User function program integrated in the program is described in gVegasFunc.cu. The calling sequence of user functions is

\[
\text{float func(float* rx, float wgt)}
\]

where \( rx \) includes a set of variables and \( wgt \) is a function weight.

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Appendix A.2 Internal programs

The gVEGAS consists of the following programs which are included in the sample codes:

- **gVegas.cu**: main program of gVEGAS system
- **gVegasCallFunction.cu**: kernel program which runs on GPU called from gVegas.cu.
- **xorshift.cu**: random number generator on GPU

Appendix A.3 Header files

The following header files which are necessary for the gVEGAS system are also included in the sample codes:

- **gvegas.h**: includes `nBlockSize` which user can set in **gVegasMain.cu**
- **vegasconst.h**: includes internal constants which are located at constant memory of GPU
- **vegas.h**: includes internal gVEGAS parameters
- **kernels.h**: a list of kernel programs which are included at CUDA compilation.

References

1. K. Hagiwara, J. Kanzaki, N. Okamura, D. Rainwater and T. Stelzer, Eur. Phys. J. C66 (2010) 477, eprint [arXiv:0908.4403](http://arxiv.org/abs/0908.4403)
2. W. Giele, G. Stavenga and J. Winter, FERMILAB-PUB-10-025-T, Feb 2010, eprint: [arXiv:1002.3446](http://arxiv.org/abs/1002.3446)
3. G. P. Lepage, J. Comput. Phys. 27 (1978) 192.
4. S. Kawabata, Comput. Phys. Commun. 41 (1986) 127, Comput. Phys. Commun. 88 (1995) 309.
5. T. Stelzer and W. F. Long, Comput. Phys. Commun. 81 (1994) 357.
6. F. Maltoni and T. Stelzer, JHEP 0302 (2003) 027.
7. J. Alwall et al., JHEP 0709 (2007) 028.