A development of an accelerator board dedicated for multi-precision arithmetic operations and its application to Feynman loop integrals II

To cite this article: H Daisaka et al 2018 J. Phys.: Conf. Ser. 1085 052004

View the article online for updates and enhancements.
A development of an accelerator board dedicated for multi-precision arithmetic operations and its application to Feynman loop integrals II

H Daisaka\(^1\), N Nakasato\(^2\), T Ishikawa\(^3\), F Yuasa\(^3\), K Nitadori\(^4\)

\(^1\) Hitotsubashi University, 2-1, Naka, Kunitachi, Tokyo, 186-0801, Japan
\(^2\) University of Aizu, Aizu-wakamatsu, Fukushima, 965-8580, Japan
\(^3\) High Energy Accelerator Research Organization (KEK), 1-1, Oho, Tsukuba, Ibaraki, 305-0801, Japan
\(^4\) RIKEN Advanced Institute for Computational Science, 7-1-26, Minatojima-minami-machi, Chuo-ku, Kobe, Hyogo, 650-0047, Japan

E-mail: daisaka@phys.science.hit-u.ac.jp

Abstract. Evaluation of a wide variety of Feynman diagrams with multi-loop integrals and physical parameters and its comparison with high energy experiments are expected to investigate new physics beyond the Standard Model. We have been developing a direct computation method of multi-loop integrals of Feynman diagrams. One of features of our method is that we adopt the double exponential rule for numerical integrations which enables us to evaluate loop integrals with boundary singularities. Another feature is that in order to accelerate the numerical integrations with multi-precision calculations, we develop an accelerator system with Field Programmable Gate Array boards on which processing elements with dedicated logic for quadruple/hexuple/octuple precision arithmetic operations are implemented. In addition, we also develop a programming interface designed for easy use of the system. The development is continued for practical use of the system. We present the current development of our system, and the numerical results of higher-loop diagrams performed using our system.

1. Introduction

The discovery of the Higgs boson in 2012 opened the door to a new era of elementary particle physics. While the Standard model has been successful, we have good enough reasons to expect new phenomena beyond it. In these investigations, precise theoretical predictions are crucial.

Recently, methods of evaluating Feynman integrals have expanded greatly in both analytic and numerical approaches. When we go into the higher order calculation, we have to include over thousands of diagrams and thus an automatic computation system is strongly required. Enormous efforts for developing such systems have been dedicated by many authors. For 1-loop integrals, several automated systems have shown successful results [1–7]. For multi-loop integrals, a lot of methods have been developed and the current status is reviewed in [8]. However, for evaluation of a wide variety of integrals including propagators with arbitrary mass scale and external momentum, there is still room for improvement.

We have been developing a fully numerical method for the evaluation of Feynman integrals which called Direct Computation Method (DCM) [9]. It is based on the numerical multidimensional integration and the extrapolation method. We can choose any kind of numerical
integration method in DCM if it gives integration results in a good enough precision. Here we use the Double Exponential Formula (DE) [10] which is one of the optimal methods in the case that there is an endpoint singularity. For the extrapolation, we use both linear and nonlinear extrapolation methods. So far, DCM have succeeded evaluating Feynman integrals with 2-, 3-, and 4-loops with 2, 3, and 4 legs [11].

However, DCM still has some difficulties for evaluating multi-loop diagrams. One is that the amount of calculation is very large, since a multi-loop diagram becomes an integration of multi-dimension. For example, a 3-loop self-energy diagram needs 7-th dimensional integration. Second is that an evaluation of multi-loop diagrams often requires calculation with high accuracy, higher than double precision, especially in the case that there is a strong singularity. Such a high accuracy calculation of Feynman loop integrals can be carried out by using high precision softwares (e.g., [12–14]). However, computation time will be much longer than the case using only double-precision. This is because in such softwares a high accuracy is realized by a combination of amount of arithmetic operations in ordinary CPUs, in other words, a large increase in operation count in the high precision case.

As one of the solutions to overcome these problems, we have been developing a dedicated accelerator system for multi-precision arithmetic operation. Based on the idea of GRAPE project (e.g., [15][16]), we have designed GRAPE-MPX architecture and the processor in which there are a number of processing elements (PE) with dedicated logic units for quadruple (hereafter MP4), hexuple (MP6), octuple-precision (MP8) arithmetic. So far, this processor has been implemented on a structured ASIC [17] and FPGAs [18]. The latest system is called GRAPE9-MPX [19][20].

In order to advance the evaluation of Feynman integrals, we continue to develop GRAPE9-MPX to have much computational power. We also continue to develop our programming interface, Goose and LSUMP, to fit to the current system, which supports the use of MPI and, furthermore, the use of GPU without changing our application program.

This paper organized as follows. The current status of GRAPE9-MPX system is explained in Section 2, and Section 3 presents the results of a 3-loop Feynman integral with two legs for the case propagators have two different mass scales as an application. The last section is dedicated for summary and discussion.

2. Overview of GRAPE9-MPX and programming interface

Figure 1 shows a schematic diagram and a picture of GRAPE9-MPX cluster system in KEK. This system is developed from the previous system with a single host and multiple FPGA boards [19][20] in order to enhance the computational power. The GRAPE9-MPX cluster system has 64 FPGA boards which are installed on 8 host computers. Each board is connected to a host via PCIe interface. For FPGA boards, we used Altera Arria V board from Intel Co. [21]. With the current implementation of our processor, the peak performance of the system achieves 403 GFlops for MP4, 185 GFlops for MP6, and 96 GFlops for MP8.

Our dedicated processor is designed by using VHDL (VHSIC Hardware Description Language) so that it is possible to implement our processor on another FPGA board, and also it is easy to make improvements. Our processor consists of two parts, MP processor and Control processor (CP). MP processor consists of PEs and broadcast memory units which form a SIMD processor. Each PE has a multiply unit, an adder unit, and register units for quadruple/hexuple/octuple-precision arithmetic. These arithmetic units perform in every clock cycle, but have 4 clock latency. Also, PE has an inverse square root (rsq) unit with a limited accuracy (19 bits for exponent and 32 bits for mantissa). This unit is used to create an initial guess for division arithmetic which is performed by Newton-Raphson method.

The role of CP is to control MP processor, by sending data and instruction necessary for calculation from a host computer to MP processor, and receiving calculation results from MP
Figure 1. Schematic diagram and picture of GRAPE9-MPX cluster system. Each host has 8 FPGA boards and is connected with GbE. For host PCs, we use Intel Xeon E5-2687W v3(6 hosts) and E5-2687W v4(2 hosts) for CPU, 128GB memory, and X10 DRX MB from SuperMicro which has 11 PCIe slots.

processor and sending them to the host. It consists mainly of IO units (including PCIe and DRAM controllers), memory components for data and instruction, and their control unit. In the current implementation, the data memory has 32k words stored on onchip memory, whereas the instruction memory has 4k words on onchip memory, and 16M words on DRAM equipped on the FPGA board.

Table 1 shows a numerical representation for MP4, MP6, and MP8 used in PE, and a specification of our dedicated processor of the current implementation. Note that we used 19 bits for exponent in order to follow IEEE binary256 format for MP8, and the same exponent is also used for MP4 and MP6 for simplicity. Our numerical representation has the total bit width 4 bits wider than a standard format used in a host computer. Therefore, we cut 4 bits from mantissa or exponent when the data is sent back to CP and a host computer. The environmental variable decides from which we cut the bits.

<table>
<thead>
<tr>
<th></th>
<th>MP4 (quadruple)</th>
<th>MP6 (hexuple)</th>
<th>MP8 (octuple)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>sign</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>Number of PE</td>
</tr>
<tr>
<td>exponent</td>
<td>19</td>
<td>19</td>
<td>19</td>
<td>Clock(MHz)</td>
</tr>
<tr>
<td>mantissa</td>
<td>112</td>
<td>176</td>
<td>240</td>
<td>Peak(Gflops)</td>
</tr>
<tr>
<td>total</td>
<td>132</td>
<td>196</td>
<td>260</td>
<td>logic utilization (%)</td>
</tr>
<tr>
<td>standard</td>
<td>128</td>
<td>192</td>
<td>256</td>
<td>mem utilization (%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>DSP utilization (%)</td>
</tr>
</tbody>
</table>

Table 1. Numerical representation (length of bit) used in PE (left), and a specification and resource utilization of our processor currently implemented in the FPGA board (right). For logic synthesis, we use Quartus 13.1 by Altera.

As already stated in [19], one of applications suited for our system is an interaction type calculation as $f_i = \sum_{j=1}^{n_j} f(X_i, Y_j)$, where $X_i$ is the $i$-th element of $X$, $Y_j$ is the $j$-th element of $Y$, and $n_j$ is the number of elements of $Y$. At calculation, data $X_i$ is set on registers in $i$-th PE, and then data $Y_j$ is sent from CP to all PEs. According to instructions sent from CP, $i$-th PE performs an evaluation of the function $f(X_i, Y_j)$ and a summation of the result. This process continues until data $X_i$ and $Y_j$ run out. In a program, this can be written as double loops. Note that a multi-dimensional integration can be expressed in double loops by using loop fusion technique that merges multiple loops into a single loop. Therefore, it is possible to accelerate a
calculation of Feynman loop integrals by using GRAPE9-MPX.

Figure 2. Schematic picture of flow of Goose and LSUMP and a sample code with the directive for a case of 1-loop box scalar integral.

Along with the development of the dedicated accelerator, we also have been developing our own compiler system, Goose and LSUMP, in order to use our system easily. Figure 2 shows the flow of compiling a program by Goose and LSUMP. Goose is a directive base compiler like OpenMP. Only procedure we have to take is to put a directive pragma (#pragma goose parallel) in an original C/C++ source code just before a double loop to be accelerated. LSUMP is our Domain Specific Language (DSL) compiler specially developed for GRAPE9-MPX. It generates a kernel executed in GRAPE9-MPX from the double loop extracted by Goose. For more detail, see Nakasato [22].

In order to use our cluster with multiple hosts and FPGA boards, we need to use a parallel computing interface such as MPI. We extended Goose to generate MPI API calls as well. In the current implementation, in the case that \( n \) hosts are used in calculation in parallel, the outer loop (\( i \)-loop) is divided into \( n \) sub loops, and each sub loop is assigned to each host. Also, we extended Goose to generate OpenCL API calls and kernels which enable us to accelerate our program by using GPGPU. For GPGPU, we use the Double-Double (DD) format [23]. Thus, by using Goose, we can accelerate our application program written in a simple C/C++ source code not only on GRAPE9-MPX but also on GPGPU with MPI.

3. Application to 3-loop Feynman integral

Here we present the numerical results of a 3-loop Feynman integral with 2 legs by DCM using GRAPE9-MPX system. Figure 3 shows a diagram of 3-loop self energy and the corresponding integral we evaluated. The number of the propagators is 8 as shown in Fig. 3 and the number of dimensions of the integration becomes 7 due to the \( \delta \)-function. The masses of the propagator are given as \( m_1 = m_2 = m_5 = m_6 = m_7 = m_8 = 1/2 \) and \( m_3 = m_4 = 1 \), in order to compare results of Ghinculov [24]. We proceeded the evaluation of the diagram by changing the kinematic variable \( p \) not only in unphysical \((0 < p^2 < 1)\) but also in physical \((1 < p^2 < 4 \) and \( 4 < p^2 \leq 8 \)) region. For the physical region, we extrapolated a resultant value from results of the integral with different values of \( p \). For the extrapolation, we used Wynn’s \( \epsilon \)-algorithm [25]. Table 2 lists a condition of calculation related to the DE formula and the extrapolation. In order to perform an integration that may be affected by singularity, we used a larger number of grids and small mesh sizes, and the extrapolation for calculations in physical region.

We computed a real part of \( I \), \( I_{re} \), in unphysical region, and both \( I_{re} \) and an imaginary part, \( I_{im} \), in physical region. Figure 4 shows the behavior of our numerical results of \( I \) as a function of \( p^2 \). There are features which should be pointed out. First feature is that \( I \) diverges at \( p^2 = 1 \) and \( 4 \). Around them, the numerical computation becomes very hard. For example,
Figure 3. 3-loop self energy diagram and the corresponding integral in a massive case we evaluated. The values $p$ and $x_i$ denote a momentum of an external line and Feynman parameters, respectively. The term $i\rho$ prevents the denominator from vanishing in the integral domain.

\begin{equation}
I = \int dx_1 dx_2 dx_3 dx_4 dx_5 dx_6 dx_7 dx_8 \frac{1}{(1 - \sum_{i=1}^{8} x_i)(D - i\rho C)^2}
\end{equation}

\begin{align*}
C &= x_3(x_3 x_{123467} + x_{123467} + x_{123467} + x_{123467}) \\
D &= -p^2 \times (x_3(x_3 x_{123467} + x_{123467} + x_{123467} + x_{123467}) \\
&\quad + x_3(x_3 x_{123467} + x_{123467} + x_{123467} + x_{123467})) \\
&\quad + x_{34}(x_3 x_{123467} + x_{123467}) \\
&\quad + x_{123467}) \\
&\quad + (m_1^2 x_1 + m_2^2 x_2 + m_3^2 x_3 + m_4^2 x_4 + m_5^2 x_5 \\
&\quad + m_6^2 x_6 + m_7^2 x_7 + m_8^2 x_8) \times C
\end{align*}

$x_{ijk...} = x_i + x_j + x_k + ...$

Table 2. Condition of calculation related to the DE formula and the extrapolation, as well as the number of FPGA boards used in calculation and precision, and elapsed time. $N$ is the number of grids per dimension, $h$ is a mesh size of the transformed variable in DE, and $\rho$ is a parameter variable used for the extrapolation.

<table>
<thead>
<tr>
<th></th>
<th>unphysical region ($I_{re}$)</th>
<th>physical region ($I_{re}, I_{im}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>25</td>
<td>64</td>
</tr>
<tr>
<td>$h$</td>
<td>0.3</td>
<td>0.0875, 0.1171</td>
</tr>
<tr>
<td>$\rho$</td>
<td>0 (fixed)</td>
<td>1.15$\beta$, $\beta = -51, -52,..., -74$</td>
</tr>
<tr>
<td>number of FPGA boards</td>
<td>1</td>
<td>64</td>
</tr>
<tr>
<td>precision</td>
<td>MP4</td>
<td>MP4</td>
</tr>
<tr>
<td>elapsed time per point</td>
<td>300 sec</td>
<td>11 hours</td>
</tr>
</tbody>
</table>

The extrapolated results, $I_{re}(p^2 = 3.99)$ is not well converged due to the severe singularity in the integration domain which causes the cancellation between positive and negative values. Second feature is that there are points which a sign for $I$ changes at $p^2 \sim 2$ and 2.5 for $I_{re}$, and $p^2 \sim 3.5$ for $I_{im}$. Last feature is that $I$ converges to zero for larger $p^2$. These features are similar to those obtained in Ghinculov [24].

Table 2 also shows the number of FPGA boards, precision used in calculation, and elapsed time per point $p$. By using our system with 64 FPGA boards, for physical region, a set of $I$ ($I_{re}, I_{im}$) with 24 different values of $\beta$ which is required for the extrapolation can be calculated in 11 hours which is acceptable. In order to increase the efficiency of calculation, we performed integrations of $I_{re}$ and $I_{im}$ with 8 different values of $\beta$ at the same time (that is, 16 integrations at the same time). The reason why such calculation is possible is that PE has registers enough to store data, and $C$ and $D$ are common so that they can be reused to save computation. The calculation time of this method is about 4 times longer than that of a single integration case in which $I_{re}$ or $I_{im}$ is individually integrated with a single value of $\beta$. Thus, in using this method, four times higher computational efficiency can be obtained.

1 The plot of $I_{re}$ and $I_{im}$ shown in Figure 5 of Ghinculov [24] seems to replace each other, because $I_{re}$ should not be zero if $p^2 < 1$. 
4. Summary and discussion
We have been developing an accelerator system dedicated for multi-precision arithmetic operators. The current system is GRAPE9-MPX cluster system with 64 FPGA boards on 8 host computers. Our dedicated processor, including PE with arithmetic logic units for MP4/MP6/MP8, is implemented on the FPGA boards. We also developed a compiler system which enables us to accelerate our application program on GRAPE9-MPX without any change in the program except for putting pragma just before double loops to be accelerated. It should be noted that the current version of Goose can generate MPI API, and OpenCL API and kernels which has the DD format, so that we can use a cluster system and GPGPU. We performed an evaluation of a 3-loop self energy diagram with mass parameters used in Ghinculov [24] and showed that our numerical method (DE-DCM + GRAPE9-MPX) can reproduce the behavior of $I$ seen in Ghinculov [24].

Note that we need to discuss about error of numerical results in Fig. 4. For unphysical region, the error is reasonable, but for physical region, the numerical error estimated from the extrapolation is 3-digit even for the best case and 1-digit for the worst case. The reason for the large error in physical region is probably due to the severe singularity appearing in the integral domain which causes large cancellation. One way to improve the accuracy is to tune parameters of the integration method, for example, increasing the number of grids and/or reducing mesh size. Another way is to divide the integral domain into sub domains and perform integration for each sub domain. In both cases, a large scale computation in multi-precision arithmetic such as quadruple/hexuple/octetuple precision will play an important role. The results will appear in future paper.

Acknowledgment
We thank Prof. Kiyoshi Kato for fruitful discussion and comments. This work is further supported by Grant-in-Aid for Scientific Research (15H03602, 15H03668, and 17K05428) of JSPS, and the Large Scale Simulation Program No. 16/17-21 of KEK.

References