Recent Developments in Parallelization of the Multidimensional Integration Package DICE
F. Yuasa\textsuperscript{a} *, K. Tobimatsu\textsuperscript{b} and S. Kawabata\textsuperscript{a}
\textsuperscript{a}High Energy Accelerator Research Organization, KEK, 1-1 OHO Tsukuba, Ibaraki 305-0801, Japan
\textsuperscript{b}Kogakuin Univ., 1-24-2 Nishi-Shinjuku, Shinjuku-ku, Tokyo 163-8677, Japan

DICE is a general purpose multidimensional numerical integration package. There can be two ways in the parallelization of DICE, “distributing random numbers into workers” and “distributing hypercubes into workers”. Furthermore, there can be the combination of both ways. So far, we had developed the parallelization code using the former way and reported it in ACAT2002 in Moscow. Here, we will present the recent developments of parallelized DICE in the latter way as the 2nd stage of our parallelization activities.

1. Introduction

Recently it is not rare to calculate the cross sections of the physics process with over 6 final state particles in the tree level. In such calculations, there may appear singularities close to diagonal integral region and sometimes it is very difficult to find a good set of variable transformations to get rid of the singularities. For the one-loop and beyond the one-loop physics processes, when we try to carry out the loop calculation only in the numerical approach, we need several multidimensional integration packages or another integration method to compare the numerical results to check them. For such a request, DICE has been developed by K. Tobimatsu and S. Kawabata. It is a general purpose multidimensional numerical integration package.

1.1. The non-parallelized version of DICE

The first version of DICE\textsuperscript{[1]} appeared in 1992 and is a scalar program code. In DICE, the integral region is divided into $2^{N_{\text{dim}}}$ hypercubes repeatedly according to the division condition. To evaluate the integral and its variance in each hypercube, DICE tries two kinds of sampling method, a regular sampling and a random sampling as:

1. Apply regular sampling and evaluate the contribution.
And then check the division condition is satisfied or not.

2. Apply 1st random sampling and evaluate the contribution.
And then check the division condition is satisfied or not.

3. Apply 2nd random sampling and evaluate the contribution.

For an integrand with singularities the number of above repetitions becomes huge so rapidly and the calculation time becomes a long time. To reduce the calculation time, the vectorized version of DICE (DICE 1.3Vh\textsuperscript{[2]}) has been developed in 1998 for vector machines. In the vector program code, the concept of workers and the queuing mechanism are introduced. This vectorized DICE has succeeded the reduction of the calculation time for the integration even when the integrand has strong singularities.

Today, however, the vector processor architecture machines have dropped off and instead the parallel processor architecture machines become common in the field of High Energy Physics. Moreover, the cost effective PC clusters running Linux with distributed memory or shared memory are widely spread. Thanks to this rapid rise
of PC clusters with the Parallel library such as MPI or with OpenMP, the parallel programming is very familiar to us.

2. Parallelization

2.1. Profile of DICE

To get a good efficiency in the parallelization, it is important to know which routines are time-consuming. UNIX command gprof is a useful tool to know it. In Table 1, an example output of gprof command for the calculation of the integration by the non-parallelized DICE. This calculation is done on the Alpha 21264 processor (700 MHz clock speed) machine running Linux and the compiler used is Compaq Fortran. In Table 1, the most time-consuming routine is elwks and is called in func. In elwk and func the integrand function is given. The subroutine func is called repeatedly in regular, random1 and random2 to evaluate the integrand. Here, vbrndm is a routine to generate random numbers and is called in both random1 and random2.

In summary, it is expected that distributing the calculations in random1 and random2 into workers (processors) may be efficient to reduce the calculation time.

2.2. Algorithm

For the integrand with strong singularities, the region is divided into a large number of hypercubes and the total number of random numbers are required to get the integral results with the requested errors. Therefore, there can be two ways in the parallelization, the way of distributing random numbers and the way of distributing hypercubes to workers.

As the 1st step we have started the parallelization of DICE with the former way, distributing random numbers. The schematic view of the algorithm with the former way is shown in Fig. 1. There, it is shown how random numbers are distributed into workers in random1 and random2. The merit of this approach is not only that the algorithm is very simple as shown in Fig. 1 but also that the overhead due to data transfer or load unbalancing among workers. The efficiency of this parallelization have showed very good performance. The result of the efficiency measurement by this parallelization way was presented at ACAT2002 at MOSCOW.

As the 2nd step, here in this paper, we present the parallelization with the latter way, distributing hypercubes into workers. As the 3rd step, the final step, we have a plan of the combination of both ways.

3. Implementation

In this parallelization, hypercubes are distributed into workers. After the evaluation, the results are gathered to the root process (for example, worker 1). And then the root process scattered the results to all workers. In Fig. 2 a schematic view how calculations are distributed into workers is shown.
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Table 1

<table>
<thead>
<tr>
<th>gprof output: Flat profile of non-parallelized DICE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time</td>
</tr>
<tr>
<td>%</td>
</tr>
<tr>
<td>82.95</td>
</tr>
<tr>
<td>12.41</td>
</tr>
<tr>
<td>2.52</td>
</tr>
<tr>
<td>0.93</td>
</tr>
<tr>
<td>0.92</td>
</tr>
<tr>
<td>0.13</td>
</tr>
</tbody>
</table>

This calculation of the integration is done on the Alpha 21264/700MHz machine by the Compaq Fortran for Linux. Total CPU time required was 9.16 sec in total. This integration was done with expected error = 10%.

4. Efficiency Measurement

4.1. Measurement Environment

In Table 2, the measurement environment is shown. There, MPI bandwidth was measured and was 56.79 MB/s. It is measured by a simple ping-pong program using MPI send-receive functions. The size of the transferred data is 1 MB and the figure is an average by 10 times measurement. In all measurements we use a cheap Gigabit Ethernet switch and it can be said that the switch showed a reasonable performance.

Table 2

<table>
<thead>
<tr>
<th>Measurement Environment: PC cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU</td>
</tr>
<tr>
<td># of systems</td>
</tr>
<tr>
<td>Memory</td>
</tr>
<tr>
<td>Switch</td>
</tr>
<tr>
<td>Compiler</td>
</tr>
<tr>
<td>MPI Bandwidth</td>
</tr>
</tbody>
</table>

4.2. Example Physics process: $e^+e^- \rightarrow \mu^+\mu^-\gamma$

We choose the radiative muon pair production as an example physics process to measure the efficiency of the parallelization. This physics process
Table 3
Summary of the parameters in the measurements

<table>
<thead>
<tr>
<th>Physics process</th>
<th>$e^+e^- \rightarrow \mu^+\mu^-\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{CM}$</td>
<td>70 [GeV]</td>
</tr>
<tr>
<td>$k_c$</td>
<td>100 [MeV]</td>
</tr>
<tr>
<td>kinematics</td>
<td>naive kinematics</td>
</tr>
<tr>
<td># of dimensions</td>
<td>4</td>
</tr>
<tr>
<td># of random numbers in each hypercube</td>
<td>100</td>
</tr>
<tr>
<td>Max. # of workers</td>
<td>8</td>
</tr>
</tbody>
</table>

is a realistic example and it must be a good example since there are several singularities in the calculation of the cross section. That is, there are the mass singularities in the initial electron and positron, those for the final muons, the s-channel singularities caused by nearly on-shell s-channel photon by a hard photon emission from the initial electron or positron, and the singularity by the infra-red divergence of a real photon which is regularized by introducing a cutoff for the photon energy $k_c$.

In Table 3, we summarized the parameters in the measurements. There we used the naive kinematics which means the kinematics without finding a good set of variables. That means there still exist several singularities in the integrand. The details of the naive kinematics are shown in Ref[2]. As a matter of course, the studies of the kinematics for this example process have been well done and we should add that there exists one program code of the kinematics with a well selected set of variables to avoid the strong singularities[3].

4.3. The Wall-Clock Time Measurement

Roughly speaking, in the parallel calculation the CPU time in each worker must decrease 1/2, 1/4, and 1/8 when the number of workers increases as 2, 4, and 8. This is the basic check whether the parallel code runs well. Actually the reduction rate of the wall-clock time is a more important measure than the reduction rate of CPU time to see how efficient the parallel code is.

In Table 4 and 5 the measured wall-clock time are shown for the calculations of the cross section with requested errors which are 1% and 2% respectively. In both Tables, the wall-clock time becomes shorter and both reduction rates are in the same manner. However, the reduction rate is not good enough when the number of workers increases.

5. Summary and Outlook

We presented recent developments on the parallelization of DICE. The ongoing work is in the 2nd stage of our activities for the parallelization. Efficiency of the current parallel code has been evaluated for the example physics process $e^+e^- \rightarrow \mu^+\mu^-\gamma$ with naive kinematics. For this process, the wall-clock time was actually reduced with the current parallel code but the reduction rate is not satisfactory when the number of workers increases. So there is still some work remained to optimize the current parallel code further.

Our current code is based on the vectorized DICE, DICE 1.3vh, and in it the load balancing mechanism between workers is not included. We believe that further more reduction of the wall-clock time will be possible with applying the load balancing mechanism to our current code.

The main goal of all efforts is the parallelization using the combination of both distribution ways. After including the load balancing mechanism we will be able to enter the 3rd stage of the parallelization.

Acknowledgments

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REFERENCES

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Table 4
Efficiency of the Parallelized DICE: The calculation of the cross section with the error = 1.97%. \( \sigma = (2.5824 \pm 0.0508) \times 10^{-2} \text{ [nb]} \)

<table>
<thead>
<tr>
<th># of Processors</th>
<th>CPU time [sec]</th>
<th>wall-clock time [sec]</th>
<th>Reduction rate: CPU time</th>
<th>Reduction rate: wall-clock time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8882.03</td>
<td>8894</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>2</td>
<td>5179.62</td>
<td>6178</td>
<td>0.58</td>
<td>0.69</td>
</tr>
<tr>
<td>4</td>
<td>3308.92</td>
<td>5011</td>
<td>0.37</td>
<td>0.56</td>
</tr>
<tr>
<td>8</td>
<td>2394.34</td>
<td>4784</td>
<td>0.27</td>
<td>0.54</td>
</tr>
</tbody>
</table>

Xeon 3.06 GHz, non-parallelized DICE, required CPU time is 8704.84 sec.

Table 5
Efficiency of the Parallelized DICE: The calculation of the cross section with error = 0.91%. \( \sigma = (2.8307 \pm 0.0259) \times 10^{-2} \text{ [nb]} \)

<table>
<thead>
<tr>
<th># of Processors</th>
<th>CPU time [sec]</th>
<th>wall-clock time [sec]</th>
<th>Reduction rate: CPU time</th>
<th>Reduction rate: wall-clock time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>186682.83</td>
<td>197444</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>2</td>
<td>109401.92</td>
<td>134377</td>
<td>0.59</td>
<td>0.68</td>
</tr>
<tr>
<td>4</td>
<td>69676.01</td>
<td>108234</td>
<td>0.37</td>
<td>0.55</td>
</tr>
<tr>
<td>8</td>
<td>51056.55</td>
<td>103126</td>
<td>0.27</td>
<td>0.52</td>
</tr>
</tbody>
</table>

Xeon 3.06 GHz, non-parallelized DICE, required CPU time is 183884.34 sec.

