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Automatic Computation of Cross Sections in HEP[*)]

—— *Status of GRACE System* ——

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For the study of physics processes in High Energy Physics (HEP) automatic computation systems have been developed and are widely used nowadays. GRACE is one of such systems and it has achieved much success in analyzing experimental data. For the large scale calculation when we deal with the cross section of given by hundreds of Feynman diagrams, parallelzation, effetive symbolic manipulation, the treatment of sigularity in the numerical integration are required. The talk will describe the software design of GRACE system and computational techniques in the GRACE.

§1. Introduction

High energy experimental physics has produced excellent results thanks to the progress of the detector and the development of the accelerator with high luminosity. Accordingly, the accurate theoretical computation is required to compare experimental results with theoretical predictions. On the other hand, as the beam energy becomes higher, there appear the physics processes with many final state particles. As a matter of course the number of relevant Feynman diagrams becomes huge. This means that Feynman amplitude calculation is practically impossible when one calculates cross sections by hands.

Since the perturbative calculation in quantum field theory is well-defined, it can be realized as an automatic computation system. There appeared several systems (`CompHEP`[1)], `FeynArt/FeynCalc`[2)]) in HEP and nowadays the automatical computation of Feynman amplitudes becomes common.

We have developed an automatic computation system named GRACE.[3)] In section 2, we describe the feature of GRACE system as a concrete example of such system. In section 3, several physical archivements by GRACE are briefly explained. In setcion 4, we discuss the techiniques in GRACE from the view point of computing.

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In final section, we summerize the problem and the future plan.

§2. GRACE System

2.1. *Tree-Level*

Using GRACE, the computaion proceeds in following steps:

1. define a physics process and generate Feynman diagrams relevant to the process, [4)]
2. generate FORTRAN code for the numerical computation referring helicity amplitude library (CHANEL) [5)]
3. compute the cross section by Monte Carlo integration package (BASES), [6)]
4. simulate the events by event generation package (SPRING). [6)]

GRACE system consists of several component-programs corresponding to each step. In the first step program named **`grc`** generates diagrams. It can generate diagrams at any order of perturbation. All the resultant information on the diagram topology, particles and vertices is stored in the list-formated file. In the next step program named **`grcfort`** generates FORTRAN code including interfaces to CHANEL and BASES. In the third step, two programs **`integ`** and **`spring`** are produced. Before proceeding to the third step we have to care about kinematics for the phase space integration using BASES. Running **`integ`**, the cross section is computed numerically. Since the distribution of the integrand is known in course of the integration, unweighted events are produced by **`spring`** in the last step.

In GRACE, several physics model files and kinematics library are necessary and stardard one's are built-in. User-defined model file or user's kinematics file can replace built-in files. GRACE also includes utility programs such as diagram-drawer, **`gracefig`**, and so on.

2.2. *One-Loop Level*

The important extension of GRACE is to compute the loop amplitudes automatically. As for the one-loop order, automatic computation of the processes with two final state particles ($2 \to 2$) is almost completed and some $2 \to 3$ processes are computed by GRACE. However, it is currently restricted to the electro-weak interaction.

The steps for the one-loop computation is almost same as those for the tree-level. However, extra steps are included due to new features needed for treating loop diagrams. We introduced the symbolic manipulation into GRACE to treat them and it processes the following steps:

(i) take the trace if there is a fermion line,
(ii) introduce Feynman parameters integration method,
(iii) shift a loop momentum appropriately,
(iv) drop odd orders of l,
(v) replace even orders of l as $l^\mu l^\nu \to g^{\mu\nu} l^2/n$ and so on,
(vi) contract vertex indices inside the loop in n-dimension. ($n = 4 - 2\epsilon$)

In order to regularize the ultra-violet divergence and the infrared divergence, the dimensional regularization and the fictitious photon mass parameter λ are introduced into GRACE, respectively.

For the loop process program `grc` generates both relevant tree diagrams and loop diagrams at once. `grc` also generates diagrams with vertex and propagator counter terms. After generating diagrams, following steps are needed as a part of step 2. in tree-level procedure:

- Generate source program for the symbolic manipulation system, REDUCE[7] or FORM[8]. Here, the product $T^{loop}T^{tree\dagger}$ are written down in a symbolic code for each pairs of an one-loop amplitude and a tree amplitude.
- Invoke REDUCE or FORM and get FORTRAN source code.

After we get FORTRAN source code, the cross sections can be calculated with the loop library and the counter term library to deal with Feynman integral and counter terms, respectively.

2.3. *How to check the results*

The important and serious issue in automatic computation is how we can check the results. For the tree-level computation GRACE can check the gauge invariance of the results by using unitary and covariant gauge. This does not work in the loop amplitude since the structure of the numerator becomes complex. For one-loop level, we newly implemented the non-linear gauge (NLG)[9] for gauge invariance check. We take a generalized NLG fixing condition for SM:

$$\begin{aligned}\mathcal{L}_{\rm GF} = \; & -\frac{1}{\xi_W}\left|(\partial_\mu - ie\tilde{\alpha}A_\mu - ig\cos\theta_W\tilde{\beta}Z_\mu)W^{+\mu} + \xi_W\frac{g}{2}(v+\tilde{\delta}H + i\tilde{\kappa}\chi_3)\chi^+\right|^2 \\ & -\frac{1}{2\xi_Z}\left(\partial_\mu Z^\mu + \xi_Z\frac{g}{2\cos\theta_W}(v+\tilde{\epsilon}H)\chi_3\right)^2 \quad -\frac{1}{2\xi_A}(\partial_\mu A^\mu)^2 \end{aligned} \tag{2·1}$$

Using NLG gauge invariance, check has been performed for several one-loop processes.

Besides gauge invariance check we can check the self-consistency of the loop-implementation to GRACE by changing parameters $1/\epsilon$ or λ. Comparison among the results derived from independent automatic computation systems shows very good agreements.[10]

2.4. *Beyond the Standard Model*

GRACE has been extended to compute the physics processes not only in the Standard Model but also the Minimal Supersymmetric extension of the Standard Model(MSSM). Here the treatment of the Majorana particles and the fermion number clashing vertices is introduced.[11] The MSSM includes 85 particles and 3,764 vertices so that the automatic calculation becomes indispensable for the calculation of SUSY processes. Recently the complete first-order radiative corrections to the process $H^+ \to t\bar{b}$ has been calculated using 1-loop system(GRACE/SUSY/1LOOP).[12]

§3. Physics Achievements

So far GRACE system has been proved to be very powerful in computing many complicated processes with many final state particles. In the tree-level $2 \to 3$ (over 50 processes), $2 \to 4$ (about 100 processes), $2 \to 5$ ($e^+e^- \to e^-\bar{\nu}_e u\bar{d}\gamma$ [13]), and $2 \to 6$ ($e^+e^- \to b\bar{b}u\bar{d}\mu\bar{\nu}_\mu$) were computed.[14] Among them it is noteworthy that 76 $e^+e^- \to$ 4-fermion processes which take place in the energy region above W^+W^- pair threshold are computed for LEP-II experiment. These 76 4-fermion programs are combined and made them up to the program named `grc4f`.[15] The one-loop level processes such as $e^+e^- \to Z^0H$, $e^+e^- \to t\bar{t}$, $e^+e^- \to W^+\mu\bar{\nu}_\mu$, and $\gamma\gamma \to W^+W^-$ were computed.[16]

To provide a practical generator for SUSY processes at LEP-II and a linear collider, we developed `susy23` which contains 23 processes for e^+e^- physics.[17] GRACE/SUSY can be extended to include R-parity violating interactions so that the process $e^+e^- \to \nu\bar{\nu}_e d\bar{d}$ in LEP-II was calculated[18].

Recently GRACE has been applied to a process at HERA experiments(GRAPE). [19] It was the lepton pair production, both in the elastic and the deep inelastic scattering regions, $ep \to epl\bar{l}$ and $ep \to el\bar{l}X$. Some routines for the proton form factors and the structure functions have been implemented.

§4. Issues Related to Computation

The first issue is the computation time. As the physics processes treated by GRACE becomes more complicated, the computation time becomes so longer that it restircts applications of the automatic computation. Among the computing steps, the multi-dimensional Monte Carlo integration consumes a lot of computing time. The requirements for reducing the execution time, we have successfully developed the first version of parallelized GRACE by using message passing library, PVM or MPI.[20] This version of parallelized GRACE reduced the computation time drastically.[21] (SU-JI????)

The second issue is related to a treatment of singularities appearing in the multi-dimensional Monte Carlo integration. In the framework of GRACE kinematics routine used in the phase space integration is not generated automatically. The aim of kinematics routine is to find an appropriate transformation between integral variables and kinematical variables to keep away from singular behavior of amplitudes in the integral region. However, we don't know yet an algorithm good enough to deal with general singularities. To find better algorithm for sigular interals is thus another big issue and it belongs to the field of numerical integration on computer.[22]

The third issue is the symbolic manipulation.

- When we write REDUCE code naively, the short of memory often happens during processing the manipulation. In order to get rid of this, many complicated and sofisticated techniques have been introduced. However in manipulation for 1-loop of $2 \to 4$ process, it is almost impossible to perform the symbolic manipulation by REDUCE. FORM system can handle the lengthy code because FORM needs less memory and computing time than REDUCE.

- When we perform the symbolic maniplucation using REDUCE and FORM, the long expressions(more than 10,000 lines) are obtained. Then very long computing time is required in numerical integration. The effective optimization should be considered. The symbolical optimization can be possible through pattern matching because Feynman diagrams contain many common parts.

The last issue is the high precision calculation in GRACE. It is sometime required from the following reasons:

- The all vertices of SM and MSSM had been checked by gauge invariance in the quadruple precision because sometimes a contribution from an amplitude changes drastically in a phase space point and it affects deeply the result. Such behavior can not be detected in our gauge invariance scheme if we use the double precision. With different gauge parameters, the relative error of the amplitude should be less than 10^{-30}.
- Due to several kinematical reasons the accuracy of numerical values may be lost. For instance, the two photon process has drastic numerical cancellation between Feynman diagrams. It may give a wrong result if one uses the double precision (10^{-15}).
- In the cross section formula, there can be a term $(W/m_e)^2$ which is $\sim 10^{+14}$ in TeV collisions where m_e is the electron mass and W is C.M. energy. This indicates that double precision is no more enough in HEP computation. In loop calculation one will loose some accuracy in the evaluation of loop integrals in additions to kinematics. In some case the calculation with full quadruple precision will be required.

§5. Summary

We have developed GRACE, an automatic computation system in HEP, and it has made much success for the study of physics process in tree and one-loop order. In the course of study, we have confronted problems of large scale computations that prevent the application of the system. The restriction can be removed by the hardware development and software engineering. Among them, we have discussed here the parallel computation, the singular integral in numerical computation, the symbolic manipulation and the floating number with high precision. Armored with those items, we can obtain the theoretical predictions for a larger class of phsical processes in the current and future accelerator projects.

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