Towards a Complete Feynman Diagrams Automatic Computation System

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Abstract:

Complete Feynman diagram automatic computation systems are now coming of age after many years of development. They are made available to the high energy physics community through user-friendly interfaces. Theorists and experimentalists can benefit from these powerful packages for speeding up time consuming calculations and for preparing event generators. The general architecture of these packages is presented and the current development of the one-loop diagrams extension is discussed. A rapid description of the prominent packages and tools is then proposed. Finally, the necessity for defining a standardization scheme is heavily stressed for the benefit of developers and users.

Invited talk at the Fourth International Workshop on Software Engineering and Artificial Intelligence for High Energy and Nuclear Physics.
AIHENP-95
Pisa April 3-8 1995
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Complete Feynman diagram automatic computation systems are now coming of age after many years of development. They are made available to the high energy physics community through user-friendly interfaces. Theorists and experimentalists can benefit from these powerful packages for speeding up time consuming calculations and for preparing event generators. The general architecture of these packages is presented and the current development of the one-loop diagrams extension is discussed. A rapid description of the prominent packages and tools is then proposed. Finally, the necessity for defining a standardization scheme is heavily stressed for the benefit of developers and users.

1. Introduction

Since its introduction by R.P. Feynman in 1949, the diagrammatic technique of computing matrix element and consequently, all physics quantities in high energy physics (HEP) has been extensively used and has proved to be the most simple, intuitive and general method to compute even the most complex processes. For its conciseness and its pictorial approach, this method has spread over other research field like atomic, nuclear and solid state physics.

Once the Lagrangian of the theory is selected, a process (defined by the initial and final state particles and the order of the calculation) is decomposed into a set of sub-processes represented by a diagram (fig.1). The real power of the Feynman approach lies, through the use of definite rules, on a quasi-mechanical transformation of each diagram in an algebraic expression representing its quantitative contribution to the process. Finally, the total cross-section is obtained by the integration over the phase space of the square of the sum of the contribution of all individual graphs. Although this approach is straight forward in its principles, the actual computation of all but the most simple processes is a quite lengthy task, prone to errors and mistakes. In order to avoid these pitfalls, calculus were used to be performed independently by several theorists until the results did fully agree. In 1967 M. Veltman wrote the first computer language to perform algebraic computation of the trace expressions resulting from the Feynman diagrams method. Schoonschip was the first step towards an automatization of these quite involved computations. For solving this same HEP computation problems, several other developments started at this time: Reduce, Macsyma. Nowadays general purpose computer algebra languages have been put on the marketplace. They provide valuable tools to per-
form many physics calculations\textsuperscript{†}: Reduc\textsuperscript{7}, Maple\textsuperscript{8}, Mathematica\textsuperscript{9}. However, the original Schoonschip and its more modern implementation, the Form language\textsuperscript{10} (J. Vermaseren) are still preferred for these specialized computations. The technique developed by R.P. Feynman is well structured and quite suited to a complete automatization. However the idea of building a complete package performing the computation of any given process only from general principles appeared to many as an enormous task and a never ending enterprise. But several groups out-passing these arguments decided to launch such projects. This workshop series has played a positive role in the motivation and the building of collaboration between these groups. Today, several packages can be used by experimentalists to create (yet with some limitations) their own event generator in an almost automatic way. Tools and libraries have also been created to facilitate complex calculations.

2. Motivations

These packages which could have remained at the level of pedagogical toys, have attracted a lot of interest because modern HEP research requires the calculation of more and more complex processes.

2.1. Larger center of mass energy

The center of mass energy of the colliders going up (LEP-II, HERA, LHC and NLC), new heavy particle thresholds (W, Z, top, Higgs) are crossed increasing therefore the number of diagrams and the level of complexity of each diagram computation.

\textsuperscript{†}P. Nason’s paper in these proceedings
2.2. Better accuracy

High precision experiments require high precision theoretical predictions. $e^+e^-$ colliders experiments belong to this category and channels bearing small contributions must be included in the computation to cope with the high statistic data. For example, the t-channel in the $e^+e^- \rightarrow ll\gamma\gamma$ where intriguing event accumulation for large $M_{\gamma\gamma}$ was observed in L3. The contribution of the non-resonant t-channels in the W production at LEP-II, often neglected, must be computed below and well above the W-pair threshold. Higher precision also means including loops diagrams as for the luminosity measurement at LEP-I which is limited by the theoretical uncertainty of the 2-loop calculation of the Bhabha scattering ($\Delta_{th} \approx 0.25\%, \Delta_{exp} \approx 0.07 - 0.16\%$). The g-2 experiments requires the computation of 4-loops contributions to barely match the experimental precision. Loop calculations are more involved than tree level ones as the n-dimensional regularization technique must be applied to treat the singularities. Furthermore, better accuracy imposes often to take into account fermion mass effects, radiative corrections and polarization effects.

2.3. More Processes

Looking for small effects revealing possible deviations from the standard model leads to the precise computation of many more processes: the "background processes", of no great theoretical importance but whose contribution could dilute or completely wash out the expected signal. Furthermore in the so-called supersymmetric models, the final state particles are often unstable ($\tilde{q} \rightarrow q + \tilde{\gamma}, \tilde{\chi}^+ \rightarrow \tilde{\chi}^0 + W^+ \rightarrow \tilde{\chi}^0 q\bar{q}$) and therefore the actual processes are rather complex (2$\rightarrow$ 4, 6 or more particles). Due to the particle inflation, more propagators are present. For example, $e^+e^- \rightarrow e^+e^- \tilde{\chi}^0 \tilde{\chi}^0$ includes 704 diagrams not taking into account the $\tilde{\chi}^0$ decay. Moreover, there are many possible models and each process may need to be computed for each model.

2.4. Perturbative QCD

Next to leading order QCD computations are highly needed for a precise comparison with the experiments, but the complexity of loop calculation in non-abelian gauge theories bridles this expectation. New methods beyond the conventional Feynman diagrammatic techniques are being developed including spinor helicity methods, supersymmetry Ward identities or string-based techniques. The inclusion of these new approaches in automatic computation packages is the next logical step.

In summary, each diagram computation gets more complex (polarization, mass effects, loops), each process gets more diagrams (loops, non-standard models, non-resonant channels), for each model, more processes (background processes,..) must be computed and finally more models have to be investigated. Therefore the need for automatic Feynman computation packages is clear as this task is beyond the reach of the theorist community.
3. Components of an Feynman diagrams automatic computation package

The general structure of a typical package is represented in the fig. 2.

3.1. Model definition

The framework on which the computation takes place has to be precisely and uniquely defined. In principle the selection of the Lagrangian should lead to the specification of all coupling constants. All fundamental parameters are computed from a set of experimental values. Several models have already been implemented, including QED, QFD, QCD and MSSM\(^1\). For example, QFD can be defined\(^2\) from a selection of the following parameters (\(\alpha(0), \alpha(Q^2), \alpha_s(Q^2), M_Z, \Gamma_Z, M_W, \Gamma_W, G_F, \sin^2 \theta_w, V_{CKM}^{ij}, M_H, M_f\)) depending essentially on the experimental precision. The coupling parameters can be computed (\(Q_f^f, g_f^f, g_f^W, g_{WWZ}\)) as well as \(M_W\) and \(\Gamma_W\) the W propagator mass and width. Then the final observables (\(|R|^2, \frac{d\sigma}{d\cos \theta}, \sigma_{tot}\)) should be uniquely defined.

3.2. Process definition

The initial and final state particles are selected as well as the order in the coupling constant (\(\alpha, g, \alpha_s\)). For example: \(e^+e^- \rightarrow W^+W^-\gamma\) at \(\mathcal{O}(\alpha^3)\) for tree level or \(e^+e^- \rightarrow W^+W^-\) at \(\mathcal{O}(\alpha^4)\) for 1 loop corrections. The final state can be generic like \(e^+e^- \rightarrow 4\) fermions or \(\gamma\gamma \rightarrow q\bar{q}\). The initial state may contain composite particles as in \(P\gamma \rightarrow P\gamma\). The way to handle radiative correction (ISR, soft photon contribution) and structure functions should also be defined.

3.3. Graph generation, drawing and selection

At the tree level, the graph generation is straightforward, the generalization to the n-loop case has been solved by the so-called "orderly algorithm"\(^3\) where all possible topologies without duplication are identified. However the computing time at a given order \(\mathcal{O}(\alpha^n)\) is proportional to the \#nodes\(^4\). Performance improvement for complex events has been achieved\(^5\) based on the use of vertex classification.

The graph drawing module, producing usually postscript diagram representation, is needed for visual check, interactive selection and inclusion in publication. This work of art has been completed in some cases up to 2-loop diagrams where topology difficulties becomes quite substantial.

Diagram ordering or classification based on some physics interest is a very important issue. Finding rules based on topological informations and model properties to select gauge invariant graph subgroups or to order diagrams by their expected contributions would provide ways to reduce computation loads.

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\(^1\) Quantum Electro Dynamic, Quantum Electroweak Dynamic, Quantum Chromo Dynamic and Minimal Supersymmetric Standard Model

\(^2\) LEP-II workshop proposal (see R. Kleiss’s talk)

\(^3\) A node is an external particle or a vertex
3.4. Matrix element elaboration

Having generated all the diagrams and using the model description, one can now write the matrix element function. It will provide the contribution of all selected diagrams for each phase space point. Two approaches are possible and have been used. Let us consider, for example, the inclusive reaction, $e^+e^- \to X$. The matrix element can be written as follows:

$$|R|^2 = \sum_{\xi, \xi'} |\bar{v}(\ell', \xi') \vartheta u(\ell, \xi)|^2$$  (1)

where $\xi, \xi'$ are helicities and $g$ graphs.

The symbolic approach

$$|R|^2 = \sum_{g, g'} \sum_{\xi, \xi'} (\bar{v}(\ell', \xi') \vartheta u(\ell, \xi)) (\bar{v}(\ell', \xi') \vartheta u(\ell, \xi))^*$$  (2)

$$|R|^2 = \sum_{g, g'} Tr(\rho' \vartheta_g \rho \vartheta_{g'}) \text{ where } \vartheta = \gamma^0 \gamma^1 \gamma^0$$  (3)

is based on trace calculus using symbolic manipulation languages: Schoonschip, Reduce, Form, Maple, Mathematica. The sum of the trace for all graphs is performed after summing over the helicities of the external particles. This technique leads to compact expressions for simple processes and to the analytic cancelation of singularities. However, large expressions are difficult to reduce (nb. terms $\propto (nb. \text{ of diagrams})^2$), polarization effect cannot easily be computed as it adds many more terms and the gauge invariant check is difficult as the computation can only been done in the most appropriate gauge scheme.

In the numerical approach, expression (1) is directly developed in wave functions, vertices and propagators components. The matrix element is then built from sequential calls to a helicity amplitude library containing all necessary numerical routines associated to each basic components. This is a systematic approach, valid for all tree level processes and not limited by the complexity of the diagrams. However, numerical stability hampers the practical use of this technique. The load is put on the integration package and its ability to deal with singularities. Large computing time is needed for the integration and event generation. For example, 100 hours on an HP-735 were necessary to compute a $(2 \to 5)$ process like $e^+e^- \to e^-\bar{\nu}_e u d\gamma$.

3.4.1. Higher order computation

Three cases should be considered: 1-loop, 2-loop and n-loop corrections. In the first case, a mixed approach (symbolic and numerical) is followed. Tree level, 1-loop diagrams and counterterms are generated, then the product of loop and tree diagrams is performed symbolically: $\Sigma_{i,j} (\text{loop})_i \ast (\text{tree})_j^*$. The output is composed of 2-4 point functions. A numerical integration is then performed using numerical\textsuperscript{17} or analytical\textsuperscript{27} scalar loop integral libraries (up-to 5-point functions). Although limited to 4 external particles in QFD, automatic computation have been used for...
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$e^+e^- \rightarrow t\bar{t}$ (2 tree and 50 1-loop diagrams) or $e^+e^- \rightarrow Z^0H$ (1 tree and 80 1-loop diagrams). Numerical instabilities and computer performance are the major limitations of this approach. Two-loop calculations is a very active field where hand computations are still necessary to find approaches suitable for automatization. These calculations imply dealing with quite complex renormalization and regularization problems. However, many tools are being developed, many partial results have been obtained and systematic approaches begin to emerge. Higher loop calculations are still in their infancy, no automatization have been yet tried, only computations with the help of algebraic tools has been achieved. Complete automation are probably impossible.$^\dagger$

3.5. Integration and event generation

The matrix element function is integrated over the multi-dimensional phase space restricted by the cuts introduced by the experimental acceptance and by the intrinsic constraints needed to tame the gauge violation divergences. The mapping of the integration parameters to the physics variable is called the kinematics. This transformation must regularize or (at least) decorrelate singularities (infra-red divergences, mass singularity, $\gamma$-t channel singularities, resonance formation) to minimize the variance in order to obtain the best numerical stability. Each singularity is mapped to an independent variable whenever possible. Otherwise, the phase space is split to adapt to each kinematical regions.

Multi-dimensional adaptive integration algorithms have been developed. In the "stratified sampling" approach, the grid spacing is adapted to the integrand magnitude and gradient (VEGAS$^{18}$, BASES$^{19}$). Iterative integration is then performed until the requested accuracy is reached.

New ideas based on quadtrees and simplexes partitioning$^{20}$ or on wavelets$^{21}$ analysis are proposed to improve the performance of this major module.

The gauge invariance is checked numerically by selecting a point in the phase space and computing the matrix element for the various gauge parameters and gauge schemes (covariant, unitary, axial gauge).

Structure functions $F(x, s)$ can be taken into account at the cost of increasing the number of dimensions in the integration $\sigma(s) = \int dx F(x, s)\sigma_0(x, s)$. The kinematics becomes also more complex due to the $s$-dependence of the integrand.

Parton shower and hadronization are performed by independent packages. The partonic final state is transformed into physical particles using one of the many hadronization scheme including: Independent fragmentation (COJET$^{22}$), Color string (JETSET/PYTHIA$^{23}$, ARIADNE$^{24}$), low-mass cluster (HERWIG$^{25}$). Color correlation and helicity constraint (resonance formation) are more difficult issues and should be implemented carefully.

Event generation is obtained by sampling the distributions computed during the integration step. SPRING$^{19}$ is an event generator which has been developed to use

$^\dagger$See D. Broadhurst’s paper in these proceedings
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4. Packages

To date\(^1\) only two packages, GRACE and COMPHEP, are fully automatic: from the process definition to the cross-section final values.

The **GRACE** packages have been developed by the Minami Tateya Collaboration.\(^2\) GRACE-T\(^2\) is a general tree level package which adopts a numerical approach based on helicity amplitudes for massive particles using the CHANEL library. The QFD and QCD model are built-in. Anomalous couplings and MSSM are almost ready to be released. Integration and event generation rely on the BASES/SPRING package. GRACE-L1 is the one-loop extension to the previous package. The generation of n-loop and counter terms is performed, but the rest of the package is limited to 1-loop and 4 external particles. Algebraic computation is performed on the product of the loop and the tree level diagrams using *Reduce*. Then a numerical integration involving scalar loop integrals is carried out. Renormalization is performed automatically in 4+\(\epsilon\) dimensions. \(e^+e^- \rightarrow t\bar{t}\) and \(\gamma\gamma \rightarrow t\bar{t}\) are some of the processes which have been calculated with this package. GRC++ is an interactive package based on KUIP embedded in PAW++. It is fully interactive for up to 2\(\rightarrow\)4 and some 2\(\rightarrow\)5 processes(fig.3).

The **COMPHEP** package has been developed by the INP Moscow Group.\(^3\) It is a general tree level system (up to 2\(\rightarrow\)4 process). It is based on an analytical approach where the square of the sum of the diagrams are computed using their own symbolic calculation package, *Reduce* or *Mathematica*. The complete QFD model is

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\(^1\)Check on these proceedings for more recent updates
treated in unitary and 'tHooft-Feynman gauge. Anomalous coupling and MSSM are in preparation. Furthermore the user may define its own model. Structure functions are implemented using PDFLIB. BASES and SPRING are used for integration and event generation. The kinematics is generated automatically for the most current needs. The package provides an interactive computation for the $2\to3$ and some $2\to4$ processes: from process specification to energy dependent total cross-sections and various angular distributions.

MADGRAPH is an automatic diagram generation package for tree level processes. It produces a matrix element in term of massless or massive helicity amplitudes using the HELAS library. The QFD and QCD model are available, MSSM will be released soon. BRS gauge invariance check is automatically built by the package. Diagram generation is interactive but the kinematics, integration and event generation are let to the user.

FEYNARTS/FEYNCALC from the Wurzburg Group is a Mathematica package providing convenient tools for radiative corrections in the Standard model. It generates and computes all tree, 1-loop graphs and some 2-loop processes. It can handle up to 4 external particles (2→2 at 1-loop and 2-loop photon self energy). QFD and QCD are basically built in and MSSM is in preparation. The 1-loop $e^+e^-\to Hz^0$ calculation has been performed with this package.

FDC, the Feynman Diagram Computation package performs automatic calculation of 1-loop diagrams using the Wick’s theorem. It follows an analytic approach based on Reduce, RLisp to produce the matrix element. This package is still in development stage.

5. Computing Aids
Some tools have been developed for more specific computations and are sometimes more advanced that some of the modules of the complete packages. However they cannot be used blindly to automatically produce cross-sections and event generators.

HIP is a high level Maple or Mathematica functions library to perform symbolic calculation on trace of product of Dirac Matrix. It provides an easy way to elaborate cross-section integrand and decay width functions. It implements the Vector Equivalence technique where pair of external fermions are replaced by an equivalent four-vector.

TRACER from the Garchin group is a Mathematica package to perform symbolic manipulation and trace operations on string of $\gamma$-algebra objects in $n$-dimensions using the 't Hooft-Veltman scheme.

COMPUTE from the Raleigh Group is a Maple or Mathematica package implementing spinor techniques for exclusive processes in perturbative QCD, for example: Nucleon Compton scattering (378 basic Feynman Diagram).

MINCER is a Form package dedicated to the calculation of massless 1, 2, 3-loop diagrams of propagator type, for example: $Z^0 \to$ Hadrons ($\alpha^3$, NNL approximation).

PHYSICA is a Mathematica package for the symbolic calculation of tree level
processes.

6. Standardization

It was decided during the workshop to set up a standardization agreement in order to open these packages to the outside world and to fix the structure of the event generators. Working groups have been formed and the PISA-I document will be available soon on http://lapphp0.in2p3.fr/aihep/aihep.html

**General package structure:** A unique definition of the input and output of each major module should permit the building of a unified workbench (Fig.4) where modules could be exchanged easily and where the same output could serve as input to several other modules.

**General structure of the event generator:** The event generator routine needs a deeper level of standardization in order to be interfaced to various structure functions, radiative corrections and hadronization packages. Moreover the general structure should permit a simple introduction in the large detector simulation packages.

7. Conclusions

Complete tree level automatic computation systems like GRACE, COMPHEP and MADGRAPH, complementary in their approaches, are available today. Improvements in the code efficiency, in the user interface and in the kinematics libraries are being pursued. Based on these packages, cross-sections and event generation databases are being prepared for all tree level processes (2 → 2, 3, 4, 5). Complete 1-loop QFD computations are close to be released. Although numerical stability problems and limitation to 4 external particles may reduce its practical use, it clearly demonstrate the feasibility of this programme and, judging from the work being dedicated to these issues, it will keep improving and getting more general in the coming years. QCD packages are now being actively developed. Next to leading order computations are investigated in the framework of supersymmetric and string based approaches. Complete automatic 2-loop correction packages are still in the science fiction section as they are one order of magnitude higher in technical complexity and in the need for computer performances. However a lot of activity is devoted to these themes and progress will definitely come. Complete automatic n-loop calculation seems out of reach with today technology. The future of automatic Feynman diagrams automatic computation depends on a widely accepted standardization scheme. Working groups have been created during this workshop to produce the first Standardization Agreement document (PISA-I) very soon.

Acknowledgments

I am happy to thank all my colleagues from the LAPP theory group, from the Minami Tateya collaboration and from the Moscow State University (INP) for their constant help and support during the preparation of this talk.
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