

Computational Physics

Monte Carlo phase space integration of multiparticle cross sections with `carlomat_4.5`

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ABSTRACT

Multidimensional phase space integrals must be calculated in order to obtain predictions for total or differential cross sections, or to simulate unweighted events of multiparticle reactions. The corresponding matrix elements, already in the leading order, receive contributions typically from dozens of thousands of the Feynman diagrams, many of which often involve strong peaks due to denominators of some Feynman propagators approaching their minima. As the number of peaks exceeds by far the number of integration variables, such integrals can practically be performed within the multichannel Monte Carlo approach, with different phase space parameterizations, each designed to smooth possibly a few peaks at a time. This obviously requires a lot different phase space parameterizations which, if possible, should be generated and combined in a single multichannel Monte Carlo procedure in a fully automatic way. A few different approaches to the calculation of the multidimensional phase space integrals have been incorporated in version 4.5 of the multipurpose Monte Carlo program `carlomat`. The present work illustrates how `carlomat_4.5` can facilitate the challenging task of calculating the multidimensional phase space integrals.

1. Introduction

Various aspects of the theory of fundamental interactions, such as the non-Abelian nature of gauge symmetry group or the mechanism of the symmetry breaking can be studied in high energy colliders through observations of processes of a few heavy particle production at a time which, if combined with their almost immediate decays, lead to multiparticle final states. In order to fully investigate the nature and interactions of the heavy particles produced, the corresponding multiparticle reactions must be measured, including their distributions and spin correlations. Such measurements can be best performed in a clean experimental environment of the planned electron-positron colliders, as the Future Circular Collider (FCC-ee) [1] and Compact Linear Collider (CLIC) [2] at CERN, the International Linear Collider (ILC) [3] in Japan, or the Circular Electron-Positron Collider (CEPC) [4] in China.

Multiparticle reactions must also be measured and compared with model predictions at low energy e^+e^- colliders in order to determine more precisely hadronic contributions to the vacuum polarization through dispersion relations from the ratio $R = \sigma(e^+e^- \rightarrow \text{hadrons})/\sigma(e^+e^- \rightarrow \mu^+\mu^-)$ at the centre of mass energies below the J/ψ production threshold. The hadronic contributions to the vacuum polarization have an impact on precision of theoretical predictions for

the muon $g - 2$ anomaly and play an important role in the evolution of the fine structure constant $\alpha(Q^2)$ from the Thomson limit to high energy scales. Precision knowledge of $\alpha(m_Z^2)$ would be vital for the Giga Z option of any future e^+e^- collider.

Derivation of theoretical predictions for cross sections or asymmetries of any multiparticle reaction requires integration over a multidimensional phase space of a squared modulus of the corresponding matrix element, which often receives contributions from several dozens of thousands or even several hundreds of thousands of the Feynman diagrams. Such multidimensional integrals can be in practice calculated only with the Monte Carlo (MC) method. Whenever denominators of the Feynman propagators approach its minimum, the corresponding amplitudes may become strongly peaked. In order to obtain reliable results of the integration, those peaks must be smoothed by appropriate changes of the integration variables. However, the number of peaks in the full amplitude of the reaction usually substantially exceeds the number of variables in the corresponding differential phase space element parameterization. Therefore, the multichannel MC approach must be used, where the name *channel* refers to a single phase space parameterization which can smooth possibly a few peaks at a time. All different parameterizations must be then combined into a single parameterization that is used in the MC integration. As the number of channels is typically

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very large, the whole process of generating appropriate multichannel differential phase space parameterization must be fully automatized.

An obvious way to follow in order to map out all the peaks is to generate one subroutine containing the phase space parameterization for each individual Feynman diagram, as it was originally done in `carlomat_1.0` [5]. However, for multiparticle reactions, this approach leads to a large number of subroutines containing different parameterizations and the resulting multichannel phase space routine is huge indeed and usually difficult to compile. Needless to say that the execution time of the MC integration would also become rather long. A modification of this approach was introduced in `carlomat_2.0` [6], where several phase space parameterizations corresponding to the Feynman diagrams of the same topology were combined into a single subroutine which resulted in a substantially shorter multichannel MC integration routine. The efficiency of that approach was further improved in `carlomat_4.0` [7] by automatic inclusion of parameterizations which map away the t-channel poles and peaks due to soft and collinear photon or gluon emission. However, for some multiparticle reactions as, e.g., $2 \rightarrow 8$ particle scattering which are relevant for the associated production of the top quark pair and the Higgs or vector boson, the resulting multichannel MC kinematics routine may be still difficult to compile and would need quite a long execution time. To overcome these difficulties a different approach was proposed in `PSGen` [8], a program for generation of phase space parameterizations for the multichannel MC integration, where the phase space parameterizations of a given reaction are generated automatically according to predefined patterns which are supposed to smooth only the most relevant peaks of the matrix element. This reduces substantially the size of the multichannel MC kinematics routine which can be very fast generated and compiled and executed in a much shorter time. However, it is obvious that, as not all the peaks present in the matrix element are taken into account by `PSGen`, some loss of the MC integration convergence should be expected.

In order to facilitate the challenging task of calculating the multidimensional phase space integrals, `carlomat_4.5`, a new version of the multipurpose Monte Carlo program `carlomat` has been written. It allows to calculate the cross section either with the kinematics routine generated by `carlomat`, or with the kinematics routine generated by `PSGen_1.1`, the current version of `PSGen`, dependent on user's choice. The kinematics chosen can be automatically combined with the leading order (LO) matrix element generated by `carlomat` or with the user provided matrix element, either in the LO or in higher orders. The MC integration can be performed either with `carlos`, a plain MC integration routine of `carlomat` [5], or `VEGAS` [11] as the latter has been implemented in `carlomat_4.5`. `VEGAS` handles peaks of the integrand with an importance sampling technique which is based on appropriate adaptation of the integration grid in subsequent iterations of the integral. As the original version of `VEGAS` [11] is limited to calculation of integrals up to 10 dimensions, its Fortran source has been modified by the author of the present work so that it can also be used to calculate integrals of higher dimension. However, as it will be discussed later on in Section 3, its use may then encounter some problems.

In the present work, a few issues concerning efficiency and convergence of the MC integration will be addressed by comparing results for the cross sections of a few physically interesting multiparticle reactions that could be measured at any future high energy e^+e^- collider. The cross sections will be calculated with different phase space parameterizations generated automatically with the above described algorithms. It will also be checked to which extent different options of performing the actual MC integration, such as the initial scan of the generated kinematics channels or an adaptation of integration weights after each iteration of the integral, or the use of adaptive MC integration routine `VEGAS` influence the integration efficiency.

The article is organized as follows. Some calculational details and useful hints concerning usage of `carlomat_4.5` are given in Section 2. Section 3 contains a sample of cross sections which should illustrate

possible problems related to the calculation of multidimensional MC integrals. The conclusions are formulated in Section 4.

2. Calculational details and program usage

In this section, some details on generation of the code, preparation for running the MC program and selection of options for numerical calculation of the cross sections presented in Section 3 are given.

The user defines the reaction to be considered and chooses the way in which the phase space parameterizations should be generated by an appropriate choice of flag `ipsgen` in `carlomat.f`, the main program of the code generation package of `carlomat_4.5` [9], the current version of `carlomat`. If integer variable `ipsgen` is set to any value different from 1 then the kinematics routine will be automatically generated by `carlomat`, else, if `ipsgen=1`, then the kinematics routine should be generated by `PSGen`, in the way described below. There are a few other flags in `carlomat.f` that should be set to desired values and then the program should be run with the command

```
make code.
```

Note that the Fortran compiler to be used is chosen in a corresponding `makefile`. If `ipsgen=1` then the user should switch to `PSGen/code_generation` and run the phase generation program there, again with the command

```
make code.
```

Prior to it, some flags described in the main program `PSGen` can be selected and the phase generation patterns can be edited in file `genps.dat` in order to map peaks of the considered reaction in the best way. How those patterns are to be defined is described in detail in [8]. Note that any predefined pattern can be commented out by setting the first integer entry of the corresponding line to 0. If the width of a massive particle is set to a character variable `zero`, then the corresponding squared four momentum transfer in the Feynman propagator will be generated according to a flat probability distribution.

The MC integration is performed with the automatically generated probability density function $f(x)$ which is defined in terms of probability density functions $f_i(x)$, $i = 1, \dots, n_{\text{kin}}$, also automatically generated, in the following way

$$f(x) = \sum_{i=1}^{n_{\text{kin}}} a_i f_i(x), \quad (1)$$

where $x = (x_1, \dots, x_{n_d})$, $0 < x_i < 1$, are random numbers and weights $a_i \geq 0$, $i = 1, \dots, n_{\text{kin}}$, satisfy the condition $\sum_{i=1}^{n_{\text{kin}}} a_i = 1$. Densities $f(x)$ and $f_i(x)$ of Eq. (1) must fulfil the following normalization conditions

$$\int_0^1 d^n f(x) = \int_0^1 d^n f_i(x) = \text{vol(Lips)}, \quad (2)$$

where vol(Lips) is the total volume of the Lorentz invariant phase space of the considered reaction. Parameterizations of differential phase space elements $f_i(x)$ of Eq. (1) are generated either with `carlomat_4.5` [9] or with `PSGen_1.1` [10], the current version of `PSGen`. The actual probability density function $f_i(x)$ according to which the final state particle four momenta are generated, which are needed to calculate the corresponding matrix element or to be stored as MC events, is chosen from the set $\{f_j(x), j = 1, \dots, n_{\text{kin}}\}$ if uniformly distributed random number $\xi \in [0, 1]$ falls into the interval $a_0 + \dots + a_{i-1} \leq \xi \leq a_0 + \dots + a_i$, with $a_0 = 0$. In the present work, the corresponding LO standard model (SM) matrix element is generated by `carlomat_4.5`.

Once the code for calculation of the matrix element and the kinematics routines have been generated, the user should choose the centre of mass energies and set the desired options, by appropriately editing the main MC program `carlcom_mpi.f` in directory `carlomat_4.5/mc_computation`. Then the program can be run with the command

make -f mpi mc.

The output will be written to files `tot_i_...`, where $i=0, 1, 2, \dots, n_{\text{proc}}$ labels computational processes within the Message Passing Interface (MPI) whose number n_{proc} should be set in the first line of the makefile `mpi`.

A number of options are available in the main program `carlocom_mpi.f` which allow to better control the MC integration. One of them is governed by flag `iscan`. If `iscan=1` then the MC integral is scanned. This means that prior to the actual calculation with a large number of calls to the integrand and, e.g. 10 iterations, it is calculated in one iteration with a relatively small, say 1000, number of calls, each time with a single phase space parameterization $f_i(x)$. The latter is selected by setting $a_i = 1$ and all other weights, $j \neq i$, $a_j = 0$. Denote the rough estimate of the cross section obtained in this way by σ_i . Then weights a_i of Eq. (1) for the first iteration of the MC integral are determined according to the following formula

$$a_i = \frac{\sigma_i}{\sum_{i=1}^{n_{\text{kin}}} \sigma_i}, \quad i = 1, \dots, n_{\text{kin}}. \quad (3)$$

On the other hand, if `iscan=0` then the first iteration of the MC integral is calculated with equal weights, $a_i = 1/n_{\text{kin}}$. Another flag in `carlocom_mpi.f` is `iwadapt`. If `iwadapt=1` then the weights a_i are calculated anew after each iteration according to Eq. (3), with σ_i being a collection of all contributions to the total cross section obtained if probability density function $f_i(x)$ has been selected for calculation of the final state particle momenta. Else, if `iwadapt=0` then all the iterations of the MC integral are calculated with the weights a_i fixed at the very beginning, i.e. before the first iteration of the MC integral.

3. Some illustrative results

In this section, the efficiency of different approaches to calculation of multidimensional integrals with the MC method is examined. As illustrative examples, the LO SM cross sections of a few physically interesting multiparticle reactions, which could potentially be measured at any future high energy e^+e^- collider, are considered. In particular, cross sections of the following reactions

$$e^+e^- \rightarrow \mu^+ \nu_\mu \mu^- \bar{\nu}_\mu, \quad n_d = 8, \quad 19 \text{ diagrams}, \quad (4)$$

$$e^+e^- \rightarrow b \mu^+ \nu_\mu \bar{b} \mu^- \bar{\nu}_\mu, \quad n_d = 14, \quad 452 \text{ diagrams}, \quad (5)$$

$$e^+e^- \rightarrow b \bar{b} b \mu^+ \nu_\mu \bar{b} \mu^- \bar{\nu}_\mu, \quad n_d = 20, \quad 46890 \text{ diagrams}, \quad (6)$$

where dimension n_d of the corresponding phase space integral and the number of the LO SM Feynman diagrams are indicated on the right hand side of each reaction, are calculated. The final states of reactions (4), (5) and (6) represent relatively clean detection channels of, respectively, W^+W^- , top quark pair production and associated production of the Higgs boson and top quark pair. To enable their identification the following cuts:

$$\begin{aligned} 5^\circ < \theta(l, \text{beam}), \theta(q, \text{beam}) < 175^\circ, & \quad \theta(l, l'), \theta(q, q'), \theta(q, l) > 10^\circ, \\ E_l, E_q > 15 \text{ GeV}, & \quad E_{T_{\text{missing}}} > 15 \text{ GeV}, \end{aligned} \quad (7)$$

where l, l' stand for either μ^- or μ^+ and q, q' stand for either b or \bar{b} , are imposed.

In order to find out the optimal probability density function of Eq. (1), the proper choice of flags and the adequate MC integration routine, the results for the LO cross sections of reactions (4) and (5) at $\sqrt{s} = 360 \text{ GeV}, 500 \text{ GeV}, 800 \text{ GeV}$ and 1 TeV are collected in Tables 1 and 2, respectively. In both tables, all entries in columns 3–6 and rows with the same value of \sqrt{s} in column 1 show the cross sections calculated with different phase space parameterizations and various choices of options for the MC integration, as described in the following. Values of `ivegas/ipsgen` listed column 2 correspond to choices of the

flags described in Section 2. In particular, if the first integer in column 2, i.e. `ivegas`, is equal to 0 (1) then the integration is performed with a plane MC integration routine `carlos` (an adaptive MC integration routine `VEGAS`). The other integer in column 2 indicates whether the multichannel probability density function $f(x)$ of Eq. (1) has been generated by `carlomat_4.5` (`ipsgen=0`) or by `PSGen_1.1` (`ipsgen=1`). The two upper rows of columns 3–6 specify choices of flags `iscan` and `iwadapt`, described in Section 2, which have been used in the MC integration of cross sections listed below.

A brief inspection of Table 1 shows that the initial scan of the generated kinematic channels reduces the standard deviation of the MC integral by roughly a factor 3. The same observations holds also for the use of adaptive MC integration routine `VEGAS`. If, in addition, the weight adaptation is turned on, then the MC error is further reduced, but to much less extent. Note, however, that the combination `ivegas/ipsgen=1/0` (`ivegas/ipsgen=1/1`) with `iscan=0` and `iwadapt=0` gives a small error with an underestimation (overestimation) of the integral, which is not compatible with the other results. This is most probably because the `VEGAS` grid adaptation algorithm is accidentally caught in some kinematics channels, with practically no possibility of choosing the other channels in consecutive iterations.

Accumulated results for the LO SM cross section of reaction (4) at $\sqrt{s} = 500 \text{ GeV}$ as functions of the number of iterations are shown in Fig. 1. The results plotted in the left panel have been integrated with the probability density function $f(x)$ of Eq. (1) generated by `carlomat_4.5` and those plotted in the right panel with $f(x)$ generated by `PSGen_1.1`. In both panels, the left histogram shows the results integrated with `carlos` while the right histogram depicts the results obtained with `VEGAS` and `iscan=1` and `iwadapt=1` have been assumed. By comparing the left and right histograms in both panels of Fig. 1, we see that the `VEGAS` algorithm reduces the standard deviation in consecutive iterations much better than that of `carlos`. One should also note that the result of the first iteration in the right panel departs substantially from the results of further iterations. This is because of the fact that the $f(x)$ generated by `PSGen_1.1` does not contain mappings of all the peaks of the integrand.

Looking at Table 2, one sees that the initial scan of the generated kinematic channels reduces the standard deviation of the MC integral even more substantially than in Table 1. However, the error reduction due to the use of adaptive integration routine `VEGAS` is not as illuminating as in Table 1. In contrary, the results for $\sqrt{s} = 800 \text{ GeV}$ and $\sqrt{s} = 1 \text{ TeV}$ obtained with the use of `VEGAS` do not seem to be reliable. It looks as if the `VEGAS` grid adaptation algorithm does not work as efficiently for $n_d = 14$, as it does for $n_d \leq 10$, which it was originally designed for. This conjecture seems to be confirmed for reaction (6), the cross sections of which integrated over the 20-dimensional phase space with `VEGAS` are not reliable at all. However, it is also possible that the `VEGAS` grid adaptation algorithm does not conform well with large number of kinematics channels for reactions (5) and (6) which are selected randomly during the computation of integral. This has been confirmed by counting calls to different kinematics channels in each iteration. After a few iterations `VEGAS` keeps calling the same kinematics all the time and hence its weight approaches 1. The plain MC integration routine `carlos` seem to cope better with these problems.

Accumulated results for the LO SM cross section of reaction (5) at $\sqrt{s} = 500 \text{ GeV}$ as functions of the number of iterations are shown in Fig. 2. The results plotted in the left panel have been integrated with the probability density function $f(x)$ generated by `carlomat_4.5` and those plotted in the right panel with $f(x)$ generated by `PSGen_1.1`, in both cases with `iscan=1` and `iwadapt=1`. Again, in both panels, the left histogram shows the results integrated with `carlos` while the right one depicts the results obtained with `VEGAS`. The advantage of the adaptive algorithm of `VEGAS` over the plain MC sampling of `carlos` in reducing the standard deviation is not any more as pronounced as in Fig. 1, as expected.

Table 1

LO cross sections in fb of reaction (4) calculated with different choices of options for the MC integration, as described in the main text. Uncertainties of the last digits are given in parentheses.

\sqrt{s} (GeV)	ivegas/ ipsgen	iscan=0 iwadapt=0	iscan=1 iwadapt=0	iscan=0 iwadapt=1	iscan=1 iwadapt=1
360	0/0	111.06(45)	111.48(17)	111.16(16)	111.74(15)
360	1/0	106.10(18)	111.69(5)	111.61(4)	111.62(4)
360	0/1	111.58(42)	111.71(16)	111.65(16)	111.53(15)
360	1/1	119.66(18)	112.57(5)	111.88(4)	111.81(4)
500	0/0	70.51(44)	70.85(16)	70.42(15)	70.55(15)
500	1/0	66.87(13)	70.62(4)	70.48(3)	70.50(3)
500	0/1	70.18(40)	70.66(15)	70.67(15)	70.36(14)
500	1/1	74.79(13)	70.98(4)	70.59(3)	70.58(3)
800	0/0	31.95(31)	32.30(11)	32.25(11)	32.11(11)
800	1/0	30.38(6)	32.23(2)	32.19(2)	32.19(2)
800	0/1	31.93(28)	32.20(11)	32.23(11)	32.08(10)
800	1/1	33.24(6)	32.22(2)	32.25(2)	32.26(2)
1000	0/0	21.09(24)	20.90(8)	20.93(8)	20.89(8)
1000	1/0	19.66(4)	20.88(1)	20.89(1)	20.90(1)
1000	0/1	20.75(21)	20.87(8)	20.95(8)	20.93(8)
1000	1/1	21.59(4)	20.82(1)	20.92(1)	20.92(1)

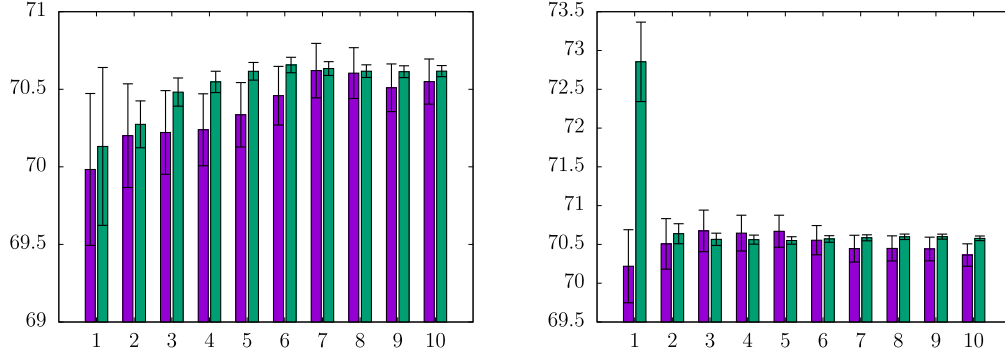


Fig. 1. Accumulated results for the LO SM cross section in fb of reaction (4) at $\sqrt{s} = 500$ GeV as functions of the number of iterations. The results plotted in the left panel have been integrated with $f(x)$ of `carlomat_4.5` and those plotted in the right panel with $f(x)$ of `PSGen_1.1`. In both panels, the left histogram has been integrated with `carlos` and the right histogram with `VEGAS`, with `iscan=1` and `iwadapt=1`.

Table 2

LO cross sections in fb of (5) calculated with different choices of options for the MC integration, as described in the main text. Uncertainties of the last digits are given in parentheses.

\sqrt{s} (GeV)	ivegas/ ipsgen	iscan=0 iwadapt=0	iscan=1 iwadapt=0	iscan=0 iwadapt=1	iscan=1 iwadapt=1
360	0/0	4.3212(222)	4.3154(25)	4.3224(31)	4.3148(23)
360	1/0	4.2001(215)	4.2509(33)	4.2989(22)	4.2991(29)
360	0/1	4.3281(123)	4.3216(25)	4.3124(17)	4.3157(19)
360	1/1	4.3497(110)	4.4967(18)	4.3337(17)	4.3234(13)
500	0/0	5.7721(334)	5.7444(45)	5.7584(52)	5.7416(45)
500	1/0	5.3242(326)	6.2811(23)	5.7385(70)	5.7384(35)
500	0/1	5.7628(173)	5.7625(28)	5.7606(30)	5.7618(26)
500	1/1	6.0091(155)	5.8128(23)	5.7627(25)	5.7644(22)
800	0/0	2.8451(214)	2.8395(56)	2.8585(93)	2.8420(68)
800	1/0	2.4527(352)	3.2007(20)	2.8013(44)	2.7906(58)
800	0/1	2.8583(91)	2.8662(20)	2.8647(22)	2.8688(20)
800	1/1	3.0329(83)	3.0706(12)	2.8634(17)	2.8625(15)
1000	0/0	1.9306(202)	1.9433(68)	1.9363(77)	1.9230(69)
1000	1/0	2.3477(276)	2.0881(9)	0.4127(430)	1.9841(50)
1000	0/1	1.9675(65)	1.9644(18)	1.9634(18)	1.9621(17)
1000	1/1	2.0288(60)	2.0864(6)	1.8903(42)	1.8667(20)

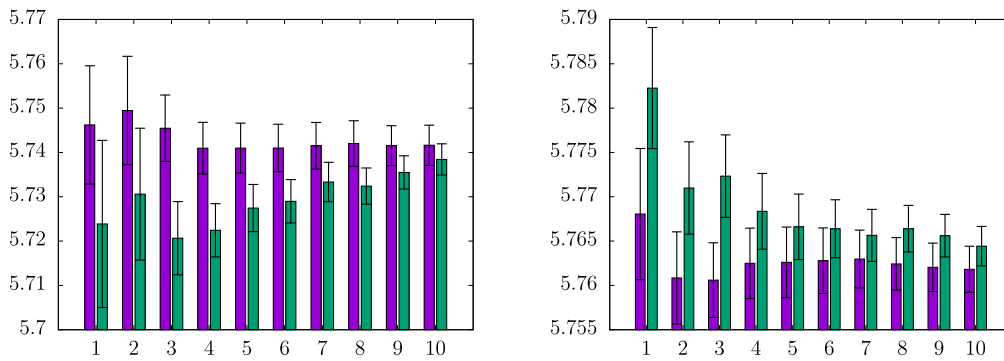


Fig. 2. Accumulated results for the LO SM cross section in fb of reaction (5) at $\sqrt{s} = 500$ GeV as functions of the number of iterations. The results plotted in the left panel have been integrated with the phase space generated by `carlomat_4.5` and those plotted in the right panel with `PSGen_1.1`. In both panels, the left histogram has been integrated with `carlos` and the right histogram with `VEGAS`, with `iscan=1` and `iwadapt=1`.

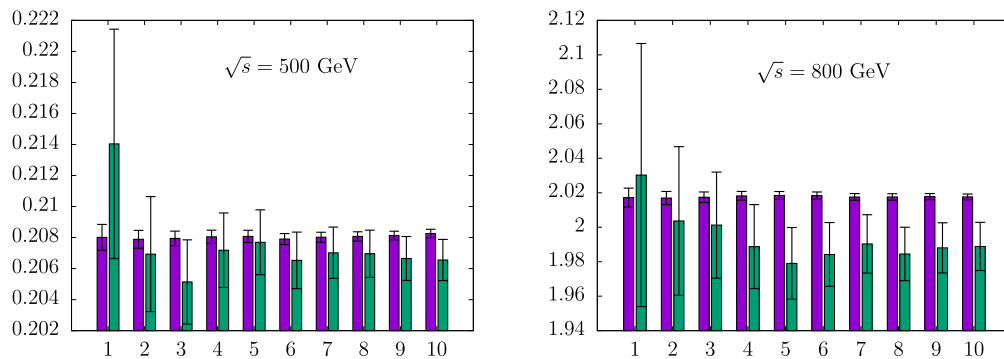


Fig. 3. Accumulated results for the LO SM cross section in fb of reaction (6) at $\sqrt{s} = 500$ GeV and $\sqrt{s} = 800$ GeV as functions of the number of iterations. The left (right) histograms in both panels have been integrated with `carlos`, using `iscan=1` and `iwadapt=1`, and the phase space generated by `carlomat_4.5` (`PSGen_1.1`).

Therefore, in Fig. 3, only the results obtained with `carlos`, using `iscan=1` and `iwadapt=1`, are shown. The accumulated results for the cross section of reaction (6) as functions of the number of iterations at $\sqrt{s} = 500$ GeV and $\sqrt{s} = 800$ GeV are plotted in the left and right panel, respectively. In both panels, the left (right) histograms show results integrated with the probability density function $f(x)$ generated by `carlomat_4.5` (`PSGen_1.1`). The advantage of the $f(x)$ of `carlomat_4.5`, which maps out all peaks of the integrand, is clearly visible. The results of consecutive iterations of the MC integral are much more stable and the standard deviation is much smaller than in case of the integration with the $f(x)$ of `PSGen_1.1` which covers only the most dominant peaks of the associated top quark pair and Higgs boson production.

4. Conclusions

It has been shown that calculation of multidimensional phase space integrals, which are necessary in order to obtain predictions for total or differential cross sections, or to simulate unweighted events of different physically interesting reactions, is a challenging task. It can be in practice solved only with the Monte Carlo method. As the corresponding matrix elements involve many peaks, the variance of the MC integral can be reduced only if those peaks are mapped out which is achieved by the use of the multichannel MC approach, with different phase space parameterizations generated and combined in the single probability distribution in a fully automatic way. A few different approaches to this task have been applied in the present work. It has been shown that there is no single golden recipe to obtain reliable results for the MC integrals of interest. Which particular approach should be used depends mostly on the dimension of the phase space integral, but also on the centre of mass energy of the considered reaction.

The Fortran code with which the results shown in the present work were obtained is public. It can be downloaded from the web pages whose addresses are given in [9], [10] and freely used.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Data availability

No data was used for the research described in the article.

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