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

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Matter To The Deepest

Recent Developments In Physics Of Fundamental Interactions

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Outline

- Motivation
- Multichannel phase space parameterization
- Automatic generation of different phase space parameterizations and adaptation of integration weights in the multichannel probability distribution
- The use of VEGAS vs plain Monte Carlo integration routine carlos
- Some illustrative results
- Summary

Based on a publication

K. Kołodziej, Computer Physics Communications **315** (2025) 109697, e-Print: 2504.00155 [hep-ph].

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- the non-Abelian nature of the SM gauge symmetry group and
- the mechanism of the symmetry breaking

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Reactions with multiparticle final states must also be taken into account if one wants to determine precisely hadronic contributions to the vacuum polarization which influences precision of theoretical predictions for the muon g-2 anomaly and plays an important role in the evolution of the fine structure constant $\alpha(Q^2)$ from the Thomson limit to high energy scales.

The hadronic contributions to the vacuum polarization can be determined through dispersion relations from the energy dependence of the ratio

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$$d^{3n_f-4}Lips = (2\pi)^4 \delta^{(4)} \Big(p_1 + p_2 - \sum_{i=3}^n p_i \Big) \prod_{i=3}^n \frac{dp_i^3}{(2\pi)^3 2E_i},$$

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Multichannel phase space parameterization

Denote i-th of N phase space parameterizations generated by

$$f_i(x) = \mathrm{d}^{3n_f-4}Lips_i(x), \qquad i=1,\ldots,N,$$

where $x = (x_1, ..., x_{3n_f-4})$ are random arguments, $x_i \in [0, 1]$. It must satisfy the normalization condition

$$\int_{0}^{1} \mathrm{d}x^{3n_f-4} f_i(x) = \mathrm{vol}(Lips).$$

All the parameterizations $f_i(x)$ are then automatically combined into a single multichannel probability distribution

$$f(x) = \sum_{i=1}^{N} a_i f_i(x),$$

with non negative weights a_i , i = 1, ..., N, satisfying the condition

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The result σ_i obtained with the *i*-th parameterization is used to calculate new weights according to the following formula

$$a_i = \sigma_i / \sum_{j=1}^N \sigma_j.$$

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Generation of the particle four momenta

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

$$\{f_j(x), j=1,...,N\}$$

if uniformly distributed random number $\xi \in [0,1]$ falls into the interval

$$a_0 + ... + a_{i-1} \le \xi \le a_0 + ... + a_i$$
, with $a_0 = 0$.

In the following, the corresponding LO SM matrix elements are generated by carlomat_4.5, but it is also possible to use higher order matrix elements generated with other programs.

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.

However, for multiparticle reactions, this approach leads to a large number of subroutines and the resulting multichannel phase space routine is huge indeed and usually difficult to compile and the execution time of the MC integration may become rather long.

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However, for some multiparticle reactions as, e.g., $2 \to 8$ 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, 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.

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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.

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Some illustrative results

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$$e^{+}e^{-} \rightarrow \mu^{+}\nu_{\mu}\mu^{-}\bar{\nu}_{\mu}, \qquad n_{d} = 8, \qquad 19 \text{ diagrams,} \quad (1)$$

$$e^+e^- \rightarrow \ b\mu^+\nu_\mu \bar{b}\mu^-\bar{\nu}_\mu, \qquad \textit{n}_{d} = 14, \qquad 452 \ \text{diagrams}, \quad (2)$$

$$e^+e^- \rightarrow \ b\bar{b}b\mu^+\nu_\mu\bar{b}\mu^-\bar{\nu}_\mu, \quad \ n_{\rm d}=20, \quad \ 46890 \ {\rm diagrams}, \quad \ (3)$$

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.

The final states of reactions (1), (2) and (3) represent relatively clean detection channels of, respectively, W^+W^- , top quark pair production and associated production of the Higgs boson and top quark pair.

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To enable their identification the following cuts:

$$\begin{split} 5^\circ < \theta(\text{I, beam}), \; \theta(\text{q, beam}) < 175^\circ, \quad \; & \theta(\text{I, I'}), \; \theta(\text{q, q'}), \; \theta(\text{q, I}) > 10^\circ, \\ E_{\text{I}}, \; E_{\text{q}} > 15 \, \text{GeV}, \qquad E_{T \, \text{missing}} > 15 \, \text{GeV}, \end{split}$$

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

 $\sigma_{LO}(e^+e^ightarrow~\mu^+
u_\mu\mu^-ar
u_\mu)$ [fb]

\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)
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)

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The initial scan reduces MC error by \sim 3.

No scan \Rightarrow results non reliable

$$\sigma_{LO}(e^+e^-
ightarrow~\mu^+
u_\mu\mu^-ar
u_\mu)$$
 [fb]

\sqrt{s} (GeV)	ivegas/ ipsgen	<pre>iscan=0 iwadapt=0</pre>	<pre>iscan=1 iwadapt=0</pre>	iscan=0 iwadapt=1	iscan=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)
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)

The initial scan reduces MC error by \sim 3.

No scan \Rightarrow results non reliable

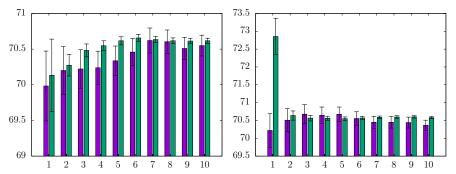
 $\sigma_{LO}(e^+e^ightarrow~\mu^+
u_\mu\mu^-ar
u_\mu)$ [fb]

\sqrt{s} (GeV)	<pre>ivegas/ ipsgen</pre>	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)
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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)

VEGAS reduces the MC error substantially. $(n_d = 8)$

$$\sigma_{LO}(e^+e^-
ightarrow~\mu^+
u_\mu\mu^-ar
u_\mu)$$
 [fb]

Accumulated results for the LO SM cross section at $\sqrt{s} = 500$ GeV as functions of the number of iterations, calculated with f(x) of carlomat_4.5 (left panel) and f(x) of PSGen_1.1 (right panel).



In both panels, the violet histogram has been integrated with carlos and the green histogram with VEGAS, with the initial scan (iscan=1) and weight adaptation (iwadapt=1).

$$\sigma_{LO}(e^+e^-
ightarrow~b\mu^+
u_\muar{b}\mu^-ar{
u}_\mu)$$
 [fb]

iccan=0

imamag/

. /c

(GeV)	ipsgen	iwadapt=0	iwadapt=0	iwadapt=1	iwadapt=1
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)

iccan-1

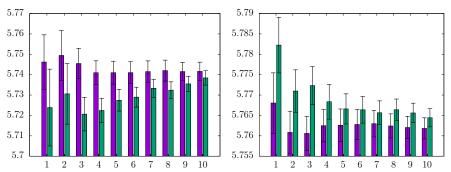
The initial scan reduces the MC error, but the use of VEGAS may give non reliable results. ($n_{\rm d}=14$)

iccan=0

iacon-1

$$\sigma_{LO}(e^+e^-
ightarrow~b\mu^+
u_\muar{b}\mu^-ar{
u}_\mu)$$
 [fb]

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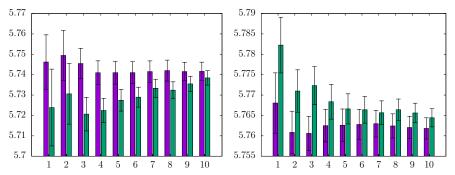


In both panels, the violet histogram has been integrated with carlos and the green histogram with VEGAS, with the initial scan (iscan=1) and weight adaptation (iwadapt=1).

The advantage of VEGAS is not clearly visible any more.

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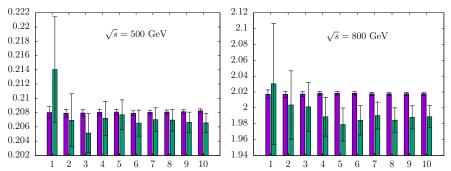
In both panels, the violet histogram has been integrated with carlos and the green histogram with VEGAS, with the initial scan (iscan=1) and weight adaptation (iwadapt=1).

The advantage of VEGAS is not clearly visible any more.

$\sigma_{LO}(e^+e^ightarrow~bar{b}b\mu^+ u_\muar{b}\mu^-ar{ u}_\mu)$ [fb]

 $n_{\rm d}=20$ \Rightarrow VEGAS does not seem applicable any more.

Accumulated results for the LO SM cross section at $\sqrt{s} = 500$ GeV and $\sqrt{s} = 800$ GeV as functions of the number of iterations:



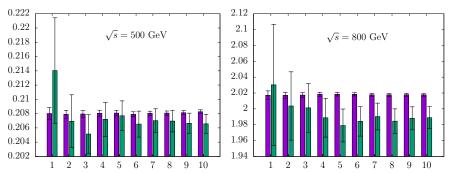
The violet histogram has been integrated with f(x) of carlomat_4.5 and the green one with f(x) of PSGen_1.1, iscan=1 and iwadapt=1 have been used.

 $n_{\rm d}=46890$, hence very many peaks are present \Rightarrow f(x) of carlomat_4.5 works better.

$\sigma_{LO}(e^+e^ightarrow\ bar{b}b\mu^+ u_\muar{b}\mu^-ar{ u}_\mu)$ [fb]

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Efficient integration of the multiparticle reaction cross sections over a multidimensional phase space is a challenge.

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.

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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.

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carlomat_4.5 and PSGen_1.1 can be useful tools to find the right solution of the problem of MC phase space integration for mutiparticle reactions.

The Fortran code with which the results shown in the present work were obtained is public. It can be downloaded from the web pages:

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