

PSGen

a generator of phase space parameterizations for the
multichannel Monte Carlo integration

Karol Kołodziej

Institute of Physics
University of Silesia

Matter To The Deepest

Recent Developments In Physics Of Fundamental Interactions

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- Motivation
- Basics of program PSGen
- Sample results
- Preparation for running and program usage
- Summary and outlook

Based on a publication K. Kołodziej, Computer Physics Communications 292 (2023) 108870 [arXiv:2303.1204[hep-ph]].

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and electron-positron colliders as

- the Future Circular Collider (FCC-ee) and Compact Linear Collider (CLIC) at CERN
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Some multipurpose programs, as [FeynArts/FormCalc](#), [GRACE](#), [MadGraph5_aMC@NLO](#), [SHERPA 2.2](#) and [HELAC-NLO](#), enable automatic calculation of the NLO EW or QCD corrections.

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Motivation

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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To obtain predictions for $e^+e^- \rightarrow \text{hadrons}$, researchers usually spend a lot of time to program necessary matrix elements by hand within some effective model and then they must invest yet more time to prepare a routine for reliable phase space integration.

Preparation of the routine for reliable phase space integration can be facilitated with a new tool, called PSGen,

which automatically generates a stand-alone Fortran 90/95 subroutine which, if called with random arguments by any MC integration routine, delivers the corresponding particle four momenta, calculated for one selected phase space parameterization, together with properly normalized differential volume element of the multidimensional phase space.

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Basics of program PSGen

The amplitudes of multiparticle reactions involve very many peaks, mostly due to denominators of the Feynman propagators, which cannot be mapped out with a single change of integration variables in the phase space integration element

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

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Phase space integration with PSGen

Denote i -th of N phase space parameterizations generated by

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

where $x = (x_1, \dots, x_{3n_f-4})$ are random arguments, $x_i \in [0, 1]$.

It must satisfy the normalization condition

$$\int_0^1 dx^{3n_f-4} f_i(x) = \text{vol}(Lips).$$

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 , $i = 1, \dots, N$, satisfying the condition

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Phase space integration with PSGen

The actual MC integration is performed with the random numbers generated according to probability distribution $f(x)$.

Integration with PSGen can be performed iteratively, as in the template program attached.

First, the MC integral is calculated N times with a rather small number of calls to the integrand, each time with a different phase space parameterization $f_i(x)$.

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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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For example, in the current version of file `genps.dat`, among others, there are the following lines:

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2 u u~ : mg,zero,  
2 e- e+ : mz,gamz.
```

The first line means that a pair of the final state quarks $u\bar{u}$ couples to the intermediate gluon of mass `mg` and width `zero` and the second line says that the e^-e^+ pair couples to the Z boson of mass `mz` and width `gamz`.

There are also entries in `genps.dat` which look like this:

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It consists of 3 final state particles $\bar{b}d\bar{u}$ which couple to two intermediate particles: the $d\bar{u}$ -quark pair couples the W boson of mass `mw` and width `gamw` and the W boson and \bar{b} -quark couple to the top quark of mass `mt` and width `gamt`.

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If the number of particles is 0, then the whole line is treated as a comment, e.g. the line

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The names of particles, their masses and widths in file `genps.dat` must conform with those listed in file `particles.dat`, where also two integers and the type of the particle in the form of `character(1)` variable at the end of each data line are given.

- The first integer specifies whether the particle couples ($= 1$) or not ($= 0$) to the photon,
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and the one character variable specifies the type of particle, *i.e.*,

- n stands for a neutrino,
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After the process has been defined, `PSGen` makes a call to the subroutine `read_process(process)`. It reads the initial and final state particles from character variable `process` and checks if all the particles are contained in data file `particles.dat` and whether they couple to the photon or gluon.

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If it is so, then `genps(nfspt)` will also generate

- the file `tchcalls.f`, which comprises calls to kinematics routines containing mappings of the t -channel poles, or
- the subroutine `kingchnl`, which contain calls to subroutines with mappings of poles due to radiation of the external photon or gluon.

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File `tchcalls.f` is included in a handwritten `subroutine kintchnl` which is located in the target directory.

Calls to `subroutines kinschnl, kintchnl and kingchnl` are all included in the `automatically generated subroutine kincls`, unless the user decides otherwise by choosing appropriate values of flags `itchnl` or `igchnl` in program `PSGen`.

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The kinematics routine

All the generated routines and auxiliary files, which are also written in Fortran 90/95, are shifted to the directory `../mc_computation`, where they are used by the kinematics routine

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subroutine psgen(ikin,ecm,x1,x2,x,ndim,flux,dlips).
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- `psgen` is self-consistent in a sense that it can be easily called by any program which integrates the S matrix element, in either the leading or higher orders of the perturbation series.

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Its automatically generated ingredients can be used in a quadruple precision version, if necessary.

The kinematics routine

All the generated routines and auxiliary files, which are also written in Fortran 90/95, are shifted to the directory `../mc_computation`, where they are used by the kinematics routine

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The particle four momenta computed in `psgen` for the kinematics `ikin` are returned in the `module fourmom` which is also created at the stage of code generation. The module is used in `psgen` and must also be used wherever the user wants to refer to the particle four momenta.

The template MC integration program

In the current distribution, `subroutine psgen` is called from a template `function cs_sect(x,ndim)`, that is integrated by a template `program PSGen_test_mpi` with the use of MC integration routine `carlos`.

- Both the routine from which `psgen` is called and the main MC integration program must include the command `use kinparams`
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Handwritten kinematics subroutines

A number of kinematics subroutines corresponding to 2, 3, ..., 9 final state particles have been written and tested.

Each of them calculates a volume of the Lorentz invariant phase space volume element and the set of the final state particle four momenta corresponding to the random arguments $x(ndim)$ they are called with.

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The user can easily add by hand a call to an own made kinematics subroutine by modifying the automatically generated subroutine `kincls` which collects calls to all kinematics subroutines of different type.

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Note, that the number of kinematics channels given by parameter `nkin` in `kinparams.f` must then be adjusted appropriately by hand according to the following formula

$$nkin = nkinag + nkinua,$$

where `nkinag` is the number of the kinematics channels automatically generated and `nkinua` is the number of channels added by the user.

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Physical input parameters

All the physical input parameters are defined in the module `inprms_ps`, located in the directory `mc_computation`, where in particular numerical values of all the particle masses and widths introduced in files `genps.dat` and `particles.dat` must be specified.

Let us compare the LO cross sections of a few reactions obtained with the MC integration of the matrix elements generated by `carlomat_4.4`, integrated with the phase parameterization based on topologies of the Feynman diagrams, as automatically generated by `carlomat_4.4`, and the phase space parameterization obtained with `PSGen`.

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Sample results

The LO cross sections at $\sqrt{s} = 0.5$ TeV and $\sqrt{s} = 1$ TeV are calculated with the cuts

$$5^\circ < \theta(l, \text{beam}), \quad \theta(\gamma, \text{beam}) < 175^\circ, \quad \theta(\gamma, l) > 5^\circ, \\ E_l > 5 \text{ GeV}, \quad E_\gamma > 1 \text{ GeV}.$$

Reaction	$\sigma(0.5 \text{ TeV})$		$\sigma(1 \text{ TeV})$	
	carlomat_4.0	PSGen	carlomat_4.0	PSGen
$e^+e^- \rightarrow b\mu^+\nu_\mu\bar{b}\mu^-\bar{\nu}_\mu$	6.565(4) fb	6.593(3) fb	2.332(8)	2.375(2) fb
$e^+e^- \rightarrow be^+\nu_e\bar{b}\mu^-\bar{\nu}_\mu$	6.624(4) fb	6.622(4) fb	2.621(11)	2.594(6) fb
$e^+e^- \rightarrow b\mu^+\nu_\mu\bar{b}\mu^-\bar{\nu}_\mu\gamma$	1.602(5) fb	1.551(11) fb	0.722(4)	0.715(5) fb

The standard deviation of the MC integration, which is given for every entry in the parentheses, is comparable for both integrations. However, **PSGen** generates much less kinematics channels than **carlomat_4.4**. This results in much shorter time of the code generation and compilation and shorter program execution time.

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Preparation for running and program usage

PSGen is distributed as a single tar.gz archive [PSGen.tgz](#) which can be downloaded from the [CPC Program Library](#) or from:

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PSGen is a new general purpose Fortran program which has been written to facilitate the Monte Carlo phase space integration of the S matrix element of any $2 \rightarrow n$ scattering process, with $n = 2, \dots, 9$, provided by the user.

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