Tutorials on Monte Carlo Integration with BASES

Junichi Kanzaki (Kavli IPMU)

Iwate Collider School 2023

@ ANA Crowne Plaza Resort Appi Kogen

February 28, 2023

Purpose of this tutorial

- We already have a great tool:
  MadGraph5_aMC@NLO which provides
  - the computations of cross-sections,
  - the event generations, and
  - the use of tools for data manipulation and analysis.
  - You should only give physics process information and some parameters.

-> This tutorial aims to help you to understand what MG5 is doing internally by experiencing calculations by yourselves.

Environment and Plan

- Environment:
  - Essential: Development with gfortran, make, ..., for the installation of BASES
  - Optional (recommended): Python3 with matplotlib for data visualization
- Plan:
  - Monte Carlo integration with BASES
    simple 1-dim., multi-dim. integration with examples of plotting.
  - Example of calculating cross-section of a physics process

Numerical Integration

- The computation of physics processes often reduces to the calculation of multivariable functions.
  - Physics quantities (ex. Cross-sections):

    $f = f(x_i, i=1 \sim N)$

    x_i: four-vectors, helicities, etc.
  - If you want to observe some quantities, $x_j, j=1 \sim n$ (p_T of lepton or jet), you must integrate other unobserved variables.
- Monte Carlo integration using random numbers is particularly useful for higher-dimensional integrals, and Monte Carlo randomly chooses points at which the integrand is evaluated.

Monte Carlo Integration (ref.)

- We already have a good lecture by Olivier this morning.

- VEGAS: G.P. Lepage, J. Comput. Phys. 27 (1978) 192–203.
- BASES: S. Kawabata, Comput. Phys. Commun. 88, 309 (1995) - Integration/Event generation
- MG5: J. Alwall, M. Herquet, F. Maltoni, O. Mattelaer, T. Stelzer, JHEP06 (2011) 128 - Integration/Event generation

Random number

- Recent random number generators have enough performance in uniformity.
- For the integrations of multi-dimensional functions, the quality of random number generation becomes essential.
- The tutorial example of BASES includes a generator based on the Mersenne Twister: https://en.wikipedia.org/wiki/Mersenne_Twister

Tutorial-0

- We assume the development environment with gfortran.
- Install python with "matplotlib" (optional) to experience plotting.
- Preparations: install libraries, bases50, helasv43, and sm
  - bases50: BASES library for the MC integration
  - helasv43: Helicity amplitude library (example4)
  - sm: Utility subroutines for the SM procces

Installation of examples

- After downloading the example package, bsexamples.tar.gz, please follow the README instruction.

```
1) Make bases libraries

   for BASES:
   cd bases50
   make install

   for HELAS:
   cd helasv43
   make install

   for other utilities:
   cd sm
   make install

   The install commands above generate the following three
libraries under ./lib:  libbases50.a, libhelasv43.a and libsm.
```

Installation of examples (cont'd)

```
2) Make examples

   cd example1
   make
   ./example1

   The program generates a histogram dump file: example1.dump

3) Test plotting (requiers matplotlib)

   ./plot.py

   This script reads contents of "example1.dump" and generates
a plot.
```

Tutorials with BASES

- Prepared samples are written in Fortran 90
- Examples are composed of the following three files:
    - mainb.f90 - main program
    - bfunc.f90 - integrand function
    - user_modules.f90 - initialization etc.

Tutorials with BASES (cont'd)

- BASES: two program phases
  - Grid optimizations
  - Data accumulations
- Parameters of BASES:
  - ncall - the number of function calls per iteration
  - it1, it2 - the maximum iterations for each program phase (it1-optimization,it2-accumulation).
  - acc1, acc2 - the accuracy to stop iterations

Tutorials with BASES (cont'd)

- In "mainb.f90" the following subroutines are called:
  call userin: initialization
  call bases: execute integration with BASES
  call bsinfo: display integration results
  call bhplot: display histograms
  call xhdump: generate histogram dump file

Tutorial-1

The integration of 1-dim. function:

$$f(x) = 2\sqrt{(1-x^2)}$$

between -1 < x < 1.

1. Make "example1" and execute it. Check the answer
2. Increase "ncall" and check the accuracy.

Tutorial-1 (cont'd)

1. Learn how to define histograms in "userin."
   call xhinit(id,xmin,xmax,nbins,title)
2. Learn how to fill histograms in "bfunc":
   call xhfill(id,val,func)
3. The program generates a histogram dump file, "example.dump." If you have "matplotlib," execute the script: plot.py, which reads the file and generates a plot.

Tutorial-2

- Another example of the integration of multi-dimensional function:

$$f(x) = \prod_{i=1}^{n_{\mathrm{dim}}} (2x_i)$$

- Try to change integration parameters.
- Try to prepare "plot.py" for the dump file, "example2.dump."

Tutorial-3

- Another example of the integration of a 2-dimensional Gaussian function:

$$f_{\mathrm{XY}}(x,y) = \frac{1}{\sqrt{2\pi\sigma_{\mathrm{X}}^2}} \mathrm{e}^{-\frac{(x-\mu_{\mathrm{X}})^2}{2\sigma_{\mathrm{X}}^2}} \times \frac{1}{\sqrt{2\pi\sigma_{\mathrm{Y}}^2}} \mathrm{e}^{-\frac{(y-\mu_{\mathrm{Y}})^2}{2\sigma_{\mathrm{Y}}^2}} .$$

- Check results and histograms.
- Learn how to define and fill 2-dimensional histograms.
- Test "plot.py" and "plot_2d.py."

Tutorial-4

Calculate cross-sections of the Standard Model physics processes: $e^-e^+ \to ZH$

$$
\begin{aligned}
\sigma &= \frac{1}{2s\beta}\frac{1}{2}\frac{1}{2}\int \sum_{\lambda} |\sum_{i} M_i|^2 d\Phi \\
\text{flux factor} &= \frac{1}{2s\beta} \\
\text{spin average} &= \frac{1}{2}\times\frac{1}{2} \\
\lambda &= \text{helicities of external particles} \\
M_i &= \text{amplitude of i-th channel} \\
\Phi &= \text{phase space}
\end{aligned}
$$

Generation of phase space

Before the calculation of amplitude of physics process, we have to generate phase space:

$$e^- e^+ \to ZH$$

W: total collision energy

m_Z: Z boson mass

m_H: Higgs boson mass

-> calculate four-vectors of external particles: p_{e^-}, p_{e^+}, p_Z, p_H

Generation of phase space

Two body phase space:

$$d\Phi_2 = \frac{1}{8\pi}\overline{\beta}(\frac{m_1^2}{s}, \frac{m_2^2}{s}) \int_{-1}^{+1} \frac{d\cos\theta}{2} \int_0^{2\pi} \frac{d\phi}{2\pi}$$

Total energy: W(=\sqrt{s}) -> $P_1(m_1)$ + $P_2(m_2)$

1. Determine energies of P_1 and P_2 (E_1 and E_2) from total energy, W

2. Determine directions (\theta and \phi) of final particles with two random numbers and calculate four momenta for P1 and P2.

   \theta: -1 < cos(\theta) < +1

   \phi: 0 < \phi < 2 \pi

Generation of phase space

Then go to three body phase space:

$$d\Phi_3 = \int_{(m_1+m_2)^2}^{(\sqrt{s}-m_3)^2} \frac{dq^2}{2\pi} \int d\Phi_2(P = q + p3) \int d\Phi2(q = p_1 + p_2)$$

$$= \frac{1}{2}\frac{1}{32\pi^2}\frac{1}{32\pi^2}\int_{(m_1+m_2)^2}^{(\sqrt{s}-m_3)^2} dq^2 \overline{\beta}\left(\frac{q^2}{s}, \frac{m_3^2}{s}\right)\overline{\beta}\left(\frac{m_1^2}{q^2}, \frac{m_2^2}{q^2}\right)$$

$$\times \int_{-1}^{+1} d\cos\theta_3 \int_0^{2\pi} d\phi_3 \int_{-1}^{+1} d\cos\hat{\theta}_1 \int_0^{2\pi} d\hat{\phi}_1$$

W(=\sqrt{s}) -> $p_1(m_1)$ + $p_2(m_3)$ + $p_3(m_3)$

-> Combination of two two-body phase space:

PS(p_3,$q=p_1+p_2$) + PS(p_1,p_2)

Generation of phase space

1. Determine the invariant mass of the system of p_1+p_2, q^2, with a random number:

$$m_1+m_2 < q^2 < W-m_3$$

2. Generate four momenta of p_3 and p_1+p_2 with two body phase space.
3. Then generate p_{10} and p_{20} at the rest frame of p_1+p_2 with q^2.
4. Rotate&Boost generated p_{10} and p_{20} to the lab. Frame, p_1 and p_2.

Tutorial-4 (cont'd)

- Requires two more libraries in addition to bases50:
  - helasv43: new helicity amplitude library
  - sm: utility library for the SM processes
- Four program components:
  - mainb.f90
  - bfunc.f90, matrix.f90, user_modules.f90

Tutorial-4 (cont'd)

- Generate a physics process with MG5 and save results with the "output standalone" command.
- Generate a physics process with MG5 and save results with the "output" command. Extract the function "matrix" part starting from:

  REAL*8 FUNCTION MATRIX(P,NHEL,IC)

  and copy it as "matrix.f90." Then, modify the character "C" at the beginning of lines to "!." Replace "INCLUDE 'coupl.inc'" with "use smcupl."

Tutorial-4 (cont'd)

- bfunc.f90:
  - generate two-body phase space: ph2bdy
  - select helicity combination as "nhel"
- As initialization in "userin":
  - call sminit - initialize SM parameters
  - call hlmode(1) - initialize the helicity amplitude library
  - initialize initial state particles

Tutorial-4 (cont'd)

1. Learn how to prepare the SM parameters.
2. Learn phase space generations.
3. Try other physics processes by yourself.
   You will learn more about how to use "MG5"!

Tutorial-5

Calculate cross-sections of the Standard Model physics processes with decays:

$$e^- e^+ \to Z(\to \mu^- \mu^+) H(\to b\bar{b})$$

1. The procedure is almost the same as "Tutorial-4."
2. Try the four-body phase space with decays.

Generation of phase space

Phase space generation for the decay of a resonance:

for the generation of the Breit-Wigner resonant shape the following variable transformation is effective.

$$x = \tan\theta$$

$$dx = d\tan\theta = \frac{1}{\cos^2\theta}d\theta = \left(1 + \tan^2\theta\right)d\theta$$

$$\rightarrow \frac{dx}{1+x^2} = d\theta = d\arctan x$$

Generation of phase space

Phase space generation for the decay of a resonance:

$$\frac{dq^2}{(q^2-m^2)^2+(m\Gamma)^2} = \frac{dq^2}{(m\Gamma)^2}\frac{1}{\left(\frac{q^2-m^2}{m\Gamma}\right)^2+1}$$

$$= \frac{1}{m\Gamma}\frac{d\frac{q^2-m^2}{m\Gamma}}{\left(\frac{q^2-m^2}{m\Gamma}\right)^2+1} = \frac{1}{m\Gamma}d\arctan\frac{q^2-m^2}{m\Gamma}$$

$$dq^2 = \frac{(q^2-m^2)^2+(m\Gamma)^2}{m\Gamma}d\arctan\frac{q^2-m^2}{m\Gamma}$$

$$= \frac{(q^2-m^2)^2+(m\Gamma)^2}{m\Gamma}d\theta$$

Generation of phase space

Phase space generation for the decay of a resonance:

$$dq^2 = \frac{(q^2-m^2)^2+(m\Gamma)^2}{m\Gamma} d\arctan\frac{q^2-m^2}{m\Gamma}$$

$$= \frac{(q^2-m^2)^2+(m\Gamma)^2}{m\Gamma} d\theta$$

$$\theta = \arctan\frac{q^2-m^2}{m\Gamma}$$

$$q^2 = m\Gamma\tan\theta + m^2$$

$$q^2_{\rm min} < q^2 < q^2_{\rm max} \Rightarrow \theta_{\rm min} < \theta < \theta_{\rm max}$$

Tutorial-5 (cont'd)

- bfunc.f90:
  - generate two-body phase space with decays: ph2dcy
    The implementation of the variable transformations in the previous pages is included in this subroutine. Please check the details.
  - You can include kinematical cuts in "bfunc.f90", which simulate the detector acceptance.

Summary

- We already have many excellent software tools for physics studies. They have much automatic functionality, which helps your analysis.
- Still, I want you to understand what procedures/technologies such software uses, not just using it
- I hope my examples help you experience the MC integration and the calculation of cross-sections and understand the calculation processes.

Summary

- If possible, try to modify these codes and test them by yourself:
  - check Ncall dependence of integration accuracies,
  - apply kinematical cuts to final state particles,
  - try other physics processes which you have some interest
  - etc.