

Monte Carlo event generators and parton showers

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Why Monte Carlo?

- ▶ Quantum mechanics are statistical in nature → measure ensembles
- ▶ Monte Carlo methods are close to how things work in “real life”

Monte Carlo Integrators :

- ▶ Simple to implement
- ▶ Handles high-dimensional integrals, even with difficult domains
- ▶ Parallilzable with trivial error estimation

General-purpose event generators (MadGraph, Pythia, Herwig, Sherpa, ...) :

- ▶ Simulate particle collisions
- ▶ Include physics models, parton showers (PS), hadronization
- ▶ Background estimation, detector simulation, etc.

Monte Carlo Markov Chains :

- ▶ Lattice QCD ($\hookrightarrow$ Justus' GRK talk)
- ▶ Fit functions in large parameter space
- ▶ Metropolis algorithm in top 10 most important algorithms of the 20th century (along Quicksort, FFT, ...)

Monte Carlo integration and convergence

Riemann sum

$$\int_a^b g(x) dx = \lim_{N \rightarrow \infty} \frac{b-a}{N} \sum_{i=1}^N g(x_i) = (b-a) \langle g \rangle$$

Monte Carlo integration with random $x_r \in (a; b)$

$$= \lim_{N \rightarrow \infty} \frac{b-a}{N} \sum_r g(x_r) = (b-a) \langle g \rangle$$

Variance, with weights $W_r = (b-a)g(x_r)$:

$$V_N(I_1) = \frac{1}{N} \sum_r (W_r - \langle W_r \rangle)^2 = \frac{1}{N} \sum_r W_r^2 - \left(\frac{1}{N} \sum_r W_r \right)^2$$

Standard deviation (via central limit theorem):

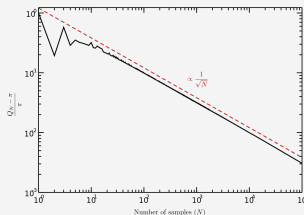
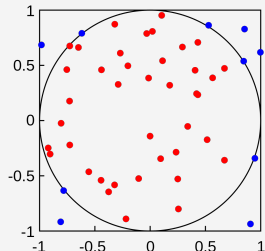
$$\sigma_N(I_1) = \sqrt{V_N(I_1)/N}$$

convergence proportional to $1/\sqrt{N}$ holds for any number of dimensions.

Simplest example: circle integration

Goal: Calculate π using Monte Carlo integration

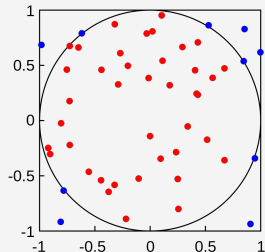
- ▶ Area of a unit circle: $A = \pi r^2 = \pi$
- ▶ $I = \int_{-1}^1 \int_{-1}^1 dx dy (1 - \theta(x^2 + y^2)) O(x, y)$
- ▶ Monte Carlo integration for area, $O = 1$:
 - ▶ Generate random points (x, y) in the square $[-1, 1] \times [-1, 1]$
 - ▶ Count the fraction of points that lie inside the circle
 - ▶ Multiply by the area of the square
- ▶ Converges as $\mathcal{O}(\frac{1}{\sqrt{N}})$ regardless of dimension



Too many dimensions

Now, moving on to a d dimensional sphere S_d in the d dimensional hypercube $C_d = [-1, 1]^d$.

Probability to hit the sphere vanishes, since the bulk of the hypercube volume is outside the sphere:



d	2	5	10	50	100
$\text{Vol}S_d/\text{Vol}C_d$	0.785	0.164	0.0025	1.5×10^{-28}	1.9×10^{-70}

$\Rightarrow$ Monte Carlo integration is not necessarily efficient at very high dimensions

Importance Sampling

We want to integrate, but it is not efficient, if g is very small in most of the integration region, since most points won't contribute much to the integral:

$$I = \int_a^b g(x) dx \quad (1)$$

Guess a function f that is similar to g to regulate the function and has a simple invertible integral F :

$$\begin{aligned} y = F(x) & \Leftrightarrow x = F^{-1}(y) \\ \frac{dy}{dx} = f(x) & \Leftrightarrow dx = \frac{dy}{f(x)} \end{aligned}$$

reduce the variance and increase the efficiency

$$I = \int_a^b g(x) dx = \int_a^b \frac{g(x)}{f(x)} dy = \int_{F(a)}^{F(b)} \frac{g(F^{-1}(y))}{f(F^{-1}(y))} dy$$

Importance Sampling

Integrate Breit-Wigner distribution¹

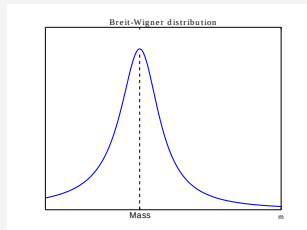
$$I = \int_{M_{\min}^2}^{M_{\max}^2} \frac{1}{(m^2 - M^2)^2 + M^2 \Gamma^2} dm^2 \quad (2)$$

Guessed transformation $m^2 \rightarrow M\Gamma \tan \rho + M^2$ gives:

$$I = \int_{M_{\min}^2}^{M_{\max}^2} \left| \frac{\partial m^2}{\partial \rho} \right| \frac{1}{(m^2 - M^2)^2 + M^2 \Gamma^2} d\rho \quad (3)$$

$$I = \int_{\rho_{\min}}^{\rho_{\max}} M\Gamma \sec^2 \rho \frac{1}{M^2 \Gamma^2 \sec^2 \rho} d\rho \quad (4)$$

$$I = \frac{1}{M\Gamma} \int_{\rho_{\min}}^{\rho_{\max}} d\rho \quad (5)$$



¹Andreas Papaefstathiou (2020). In: *Eur. Phys. J. Plus* 135.6, p. 497. arXiv: 1412.4677 [hep-ph].

Koksma-Hlawka Inequality

Statement

The Koksma-Hlawka inequality provides an upper bound on the discrepancy of numerical integration using a low-discrepancy sequence.

$$\left| \frac{1}{N} \sum_{j=1}^N f(x_j) - \int_{[0,1]^d} f(x) dx \right| \leq D_N V(f) \quad (6)$$

where f is a function on the d -dimensional unit cube $[0, 1]^d$, $x_1, x_2, \dots, x_N$ are points in $[0, 1]^d$, $D_N = \sup_{t \in [0,1]^d} \left| \frac{1}{N} \sum_{j=1}^N \chi_{[0,t]}(x_j) - \prod_{k=1}^d t_k \right|$ is the discrepancy of the point set $x_1, x_2, \dots, x_N$, and $V(f)$ is the variation of the function f and $\chi_{[0,t]}(x)$ is the characteristic function of the axis-aligned box $[0, t] = [0, t_1] \times [0, t_2] \times \dots \times [0, t_d]$.

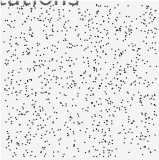
$\Rightarrow$ i.e. discrepancy compares number of points in a box to the volume of the box.

$\Rightarrow$ equidistributed sequence typically achieve convergence rates of $\mathcal{O}(\frac{\log^{d-1} n}{n})$ which are much better than the $\mathcal{O}(\frac{1}{\sqrt{N}})$ of ordinary Monte Carlo

Random Number Generation and Sequences

Mersenne Twister Pseudo-Random Numbers

- ▶ long period of $2^{19937} - 1$
- ▶ good statistical properties
- ▶ suits most general-purpose simulations and computations



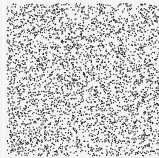
n = 1000



n = 2000



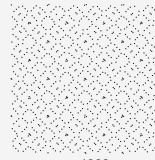
n = 3000



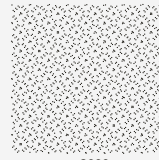
n = 4000

Sobol Quasi-Random Numbers

- ▶ well-distributed across the space
- ▶ deterministic, but not random
- ▶ avoids clustering of points



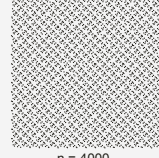
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Modern Monte Carlo Integration routines

Vegas² :

- ▶ adaptive importance sampling
- ▶ sample in hypercubes assuming separation $g(x_1, x_2, \dots) = g_1(x_1)g_2(x_2) \dots$
- ▶ adapt the size of the hypercubes to the function

CUBA³ :

- ▶ **Suave**: globally adaptive subdivision $\rightarrow$ bisection in area of largest error
- ▶ **Divonne**: stratified sampling $\rightarrow$ split up the integration region into parts with equal variance (spread), then sample all parts with same number of points.

FOAM⁴ :

- ▶ triangulation of the integration region into cells

i-flow⁵ :

- ▶ Machine learning of the importance sampling function based on normalizing flows (invertible neural networks)

²G. Peter Lepage (1978). In: *J. Comput. Phys.* 27, p. 192.

³T. Hahn (2005). In: *Comput. Phys. Commun.* 168, pp. 78–95. arXiv: [hep-ph/0404043](#).

⁴S. Jadach (2003). In: *Comput. Phys. Commun.* 152, pp. 55–100. arXiv: [physics/0203033](#).

⁵Christina Gao, Joshua Isaacson, and Claudius Krause (2020). In: *Mach. Learn. Sci. Tech.* 1.4, p. 045023. arXiv: [2001.05486 \[physics.comp-ph\]](#).

Event generation

Instead of integrating, we can also use Monte Carlo to generate events according to a given distribution.

- ▶ Collect a set of phase-space points corresponding to events
- ▶ Events need to be assigned weights according to the distribution
- ▶ Small **weighted events** are is wasteful for further processing

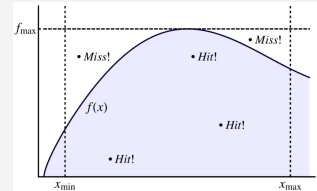
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“**hit-or-miss**” **method**, keep only events proportional to probability/weight:

- ▶ Store the maximum of the distribution $f_{\max}$ during integration for total cross section/normalization $\langle f \rangle$
- ▶ Pick phase-space points randomly and accept them with probability $f(x)/f_{\max}$
- ▶ Each accepted event gets a weight $\langle f \rangle \Rightarrow$ generates **unweighted events**
- ▶ Information about the distribution is in the number of events instead of the weight

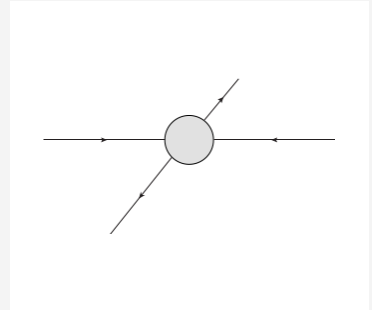


Generating full events

$$d\sigma = \sum_{a,b} \int_0^1 dx_a dx_b$$

$$\underbrace{d\hat{\sigma}_{cX}(x_a P_A, x_b P_B, \mu_F)}_{\text{partonic cross section}}$$

1. **Hard process generation:** Pick a phase space following hit-or-miss method

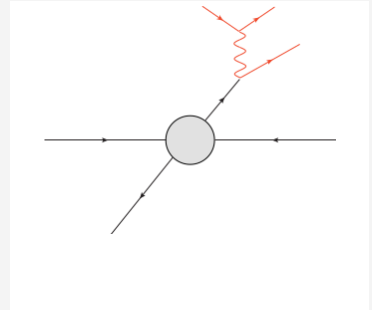


Generating full events

$$d\sigma = \sum_{a,b,c} \int_0^1 dx_a dx_b dz$$

$$\underbrace{d\hat{\sigma}_{cX}(x_a P_A, x_b P_B, \frac{P_\gamma}{z}, \mu_F)}_{\text{partonic cross section}} \underbrace{D_{Y/c}(z, \mu_F)}_{\text{fragmentation}}$$

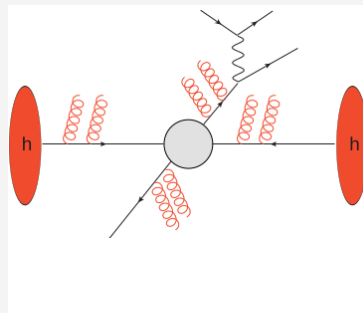
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2. **Heavy resonance decay:** Heavy resonances with narrow widths are decayed before the parton shower



Generating full events

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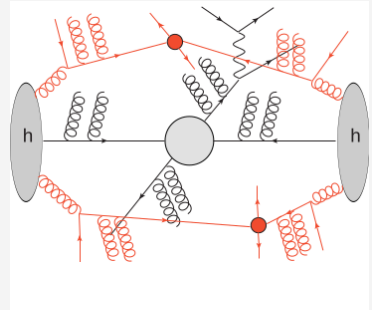
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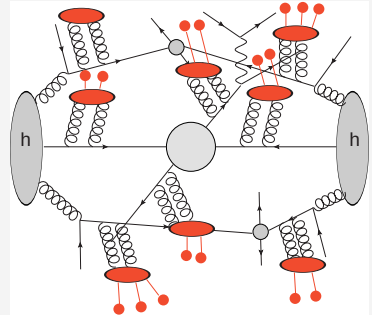
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4. **Multiple parton interactions:** Secondary interactions between partons within the colliding hadrons, modelled as QCD $2 \rightarrow 2$ interactions, are generated



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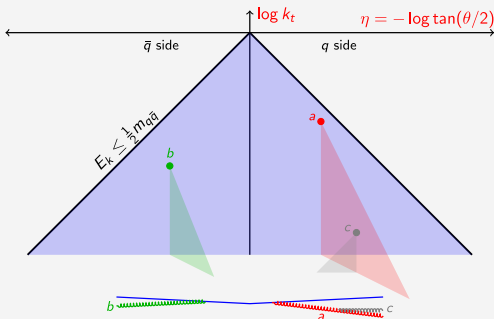
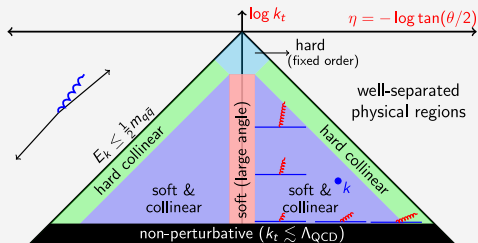
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5. **Hadronization and hadron decays:** In the cluster model, clusters are formed and hadrons are produced. Unstable hadrons are subsequently decayed.



Parton shower

soft ($k_T \rightarrow 0$) and collinear ($\theta \rightarrow 0$ or π) approximation of the DGLAP splitting probability⁶

$$d\mathcal{P}_{a \rightarrow bc} = \frac{\alpha_s(k_T)}{2\pi} \frac{dQ^2}{Q^2} P_{a \rightarrow bc}(z) dz \quad (7)$$



⁶Gregory Soyez (2023). Parton Showers and Resummations (PSR), 6-8 June 2023. URL: <https://indico.cern.ch/event/1202436/contributions/5288130/attachments/2660262/4608836/lund.pdf>.

Parton shower

Sudakov Form Factor and Leading Logarithms

Emission probability:

$$\mathcal{P}_{\text{no}}(0 \leq t < T) = \lim_{n \rightarrow \infty} \prod_{i=0}^{n-1} \mathcal{P}_{\text{no}}(T_i \leq t < T_{i+1})$$

Parton shower

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Parton shower

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Parton shower

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$$\mathcal{P}_{\text{first}}(T) = 1 - \mathcal{P}_{\text{no}}(T) \implies d\mathcal{P}_{\text{first}}(T) = d\mathcal{P}_{\text{em}}(T) \exp \left(- \int_0^T \frac{\mathcal{P}_{\text{em}}(t)}{dt} dt \right)$$

Parton shower

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In momentum space there is no $t \implies$ use $t \sim 1/Q$ (Heisenberg)

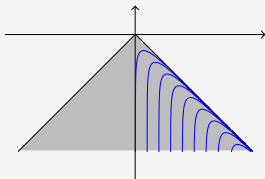
Parton shower

Angular vs k_T ordered shower

Angular ordered parton shower

$$Q^2 = E_a^2 \theta_{a \rightarrow bc}^2 \quad (8)$$

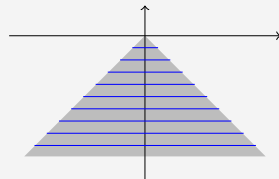
- ▶ Successive emission has a smaller angle compared to the previous one
- ▶ Small dead zone at $\ln p_T^2/\tilde{s}$
- ▶ Correct color factors for observables insensitive to azimuthal correlations



Transverse-momentum-ordered parton shower

$$Q^2 = k_T^2 \quad (9)$$

- ▶ Ordered by their transverse momentum k_T relative to their parent parton
- ▶ Resums large logarithms of the form $\alpha_s^n \ln^{2n}(M^2/k_T^2)$, with M the hard scale
- ▶ Color factors in improved leading-color approximation



Matrix Elements vs Parton Showers

Matrix Elements

- + Fixed order $\Rightarrow$ good for hard jets
- + contains all α_s terms up to a given order
- + valid for high p_T^2
- expensive to compute $\Rightarrow$ only few emissions

Parton Showers

- + Always finite
- + Any number of emission
- Only valid in soft/collinear regions

$\Rightarrow$ Combine the two to get the best of both worlds via NLO Matching or Multi-jet Merging ($\hookrightarrow$ Alex' intermediate master talk)

- ▶ Hard emissions by fixed order predictions
- ▶ Further emissions probabilities from PS

NLO Matching

Madgraph5 - MC@NLO

NLO observable

$$\begin{aligned} \langle \mathcal{O} \rangle &= \int d\phi_n (B_n + V_n) \mathcal{O}_n(\phi_n) \sim \text{hard final state} + \text{virtual radiation (loop)} \\ &+ \int d\phi_{n+1} B_{n+1} \mathcal{O}_{n+1}(\phi_{n+1}) \sim \text{real radiation} \end{aligned}$$

NLO Matching

Madgraph5 - MC@NLO

Handle divergences between B_{n+1} and V_n with universal FKS subtraction terms:

$$\begin{aligned}
 \langle \mathcal{O} \rangle = & \int d\phi_n (B_n + V_n + B_n \otimes I_1) \mathcal{O}_n(\phi_n) \sim \text{hard final state} + \text{virtual radiation (loop)} + \int \text{counter terms} \\
 & + \int d\phi_{n+1} (B_{n+1} \mathcal{O}_{n+1}(\phi_{n+1}) - B_n \otimes D_1 \mathcal{O}_n(\phi_{n+1})) \sim \text{real radiation} - \text{counter terms}
 \end{aligned}$$

Attaching a emission to the LO by the PS overlaps with Real correction:

$$PS_n \sim \text{hard final state} + \text{real radiation}$$

NLO Matching

Madgraph5 - MC@NLO

Avoid double counting between NLO and PS⁷:

$$\begin{aligned}
 \langle \mathcal{O} \rangle = & \int d\phi_n (B_n + V_n + B_n \otimes I_1) PS_n(\mathcal{O}_n, \phi_n) \sim \text{hard final state} + \text{virtual radiation (loop)} + \int \text{counter terms} \\
 & + \int d\phi_{n+1} (B_{n+1} - B_n \bar{P}_{n+1}) PS_{n+1}(\mathcal{O}_{n+1}, \phi_{n+1}) \sim \text{real radiation} - \text{counter terms} \\
 & + \int d\phi_{n+1} (B_n \bar{P}_{n+1} - B_n \otimes D_1) PS_n(\mathcal{O}_n, \phi_{n+1}) \sim \text{counter terms} - \text{counter terms}
 \end{aligned}$$

with PS :

$$\begin{aligned}
 PS_n & \sim \text{hard final state} + \text{virtual radiation (loop)} + \dots \\
 PS_{n+1} & \sim \text{real radiation} - \text{counter terms} + \dots
 \end{aligned}$$

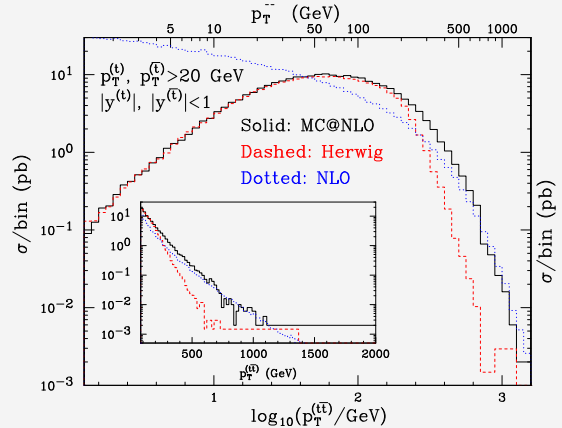
⁷ John Campbell (n.d.). URL:

<https://indico.fnal.gov/event/9650/attachments/74470/89343/MCGenerators.pdf>; Leif Gellersen (2022). CTEQ Summer School 2022. URL: <https://indico.cern.ch/event/1131319/contributions/4895915/>

NLO Matching

Madgraph5 - MC@NLO

- ▶ Smooth transition between lower and high scales
- ▶ Needs shower implementation with correct counterterms
- ▶ Regulates low p_T region
- ▶ Can lead to many events with negative weights



8

⁸Paolo Nason and Bryan Webber (2012). In: *Ann. Rev. Nucl. Part. Sci.* 62, pp. 187–213. arXiv: 1202.1251 [hep-ph].

NLO Matching

POsitive Weight Hardest Emission Generator (POWHEG)

- ▶ POWHEG attaches first emission to n -particle state with a modified Sudakov factor such that NLO accuracy is preserved.

$$\Delta_R(p_T) \sim \exp \left[- \int d\Phi_R \frac{R(\Phi_B, \Phi_R)}{B(\Phi_B)} \theta(k_T(\Phi_B, \Phi_R) - p_T) \right]$$

- ▶ Sudakov Δ_R is no emission probability. This can be seen from singular behavior as $R \rightarrow \infty$ thus the no emission probability goes to 0.

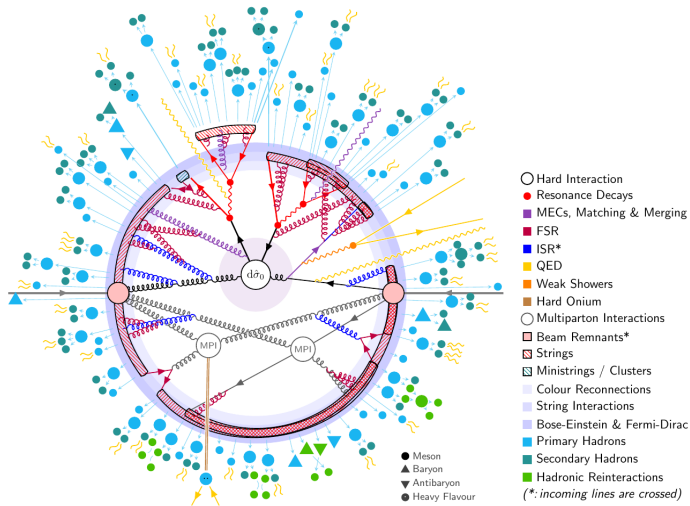
- ▶ solve for p_T with random $r \in (0, 1)$, where U is the upper bound of the Sudakov factor $f \sim \frac{R}{B}$ similar to splitting of $P_{a \rightarrow bc}$.

$$\log \Delta^U(p_T) = \log(r)$$

- ▶ accept event with $P_{\text{acc}} = f/U$ probability and reject with $1 - f/U$ probability.
- ▶ if rejected, repeat procedure for lower p_T until the emission is accepted or Λ_{QCD} is reached.
- ▶ PS must generate radiation only from below the scale k_T ($\rightarrow$ veto algorithm for angular ordered PS).

Summary

- ▶ Monte Carlo integration is a powerful tool to integrate high-dimensional integrals
- ▶ Discussed different steps from hard process to hadronization
- ▶ Consistency of NLO computation with soft-collinear parton shower can be achieved with different methods (POWHEG, MC@NLO)
- ▶ Parton showers take higher order logs and color correlations into account like resummation
- ▶ Computational cost is a limiting factor $\implies$ many possibilities to optimize the performance of the MC



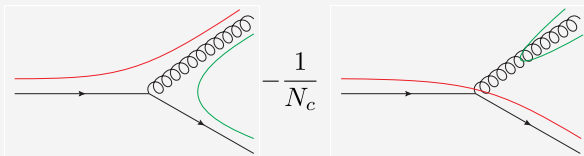
Thank you!

Leading Color Correlations

Go to the large N_c limit:

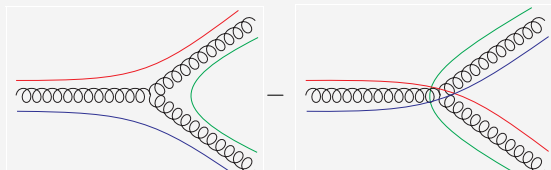
► Quark-quark-gluon vertex

$$T_{ij}^a T_{kl}^a = \frac{1}{2} \left(\delta_{il} \delta_{jk} - \frac{1}{N_c} \delta_{ij} \delta_{kl} \right) \quad (10)$$

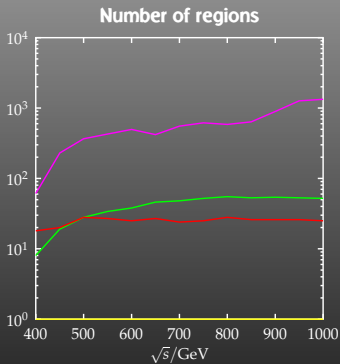
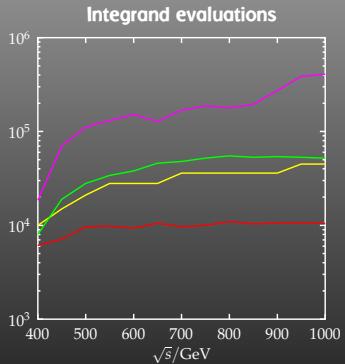


► gluon-gluon-gluon vertex

$$f^{abc} T_{ij}^a T_{kl}^b T_{mn}^c = (\delta_{il} \delta_{kn} \delta_{mj} - \delta_{in} \delta_{ml} \delta_{kj}) \quad (11)$$



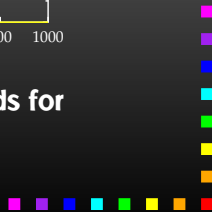
Test Run



$$e^+ e^- \rightarrow \bar{t} t \gamma$$
$$\varepsilon_{\text{rel}} = 3 \times 10^{-3}$$

Vegas
Suave
Divonne
Cuhre

Above all: Very important to have several methods for cross-checking the results!



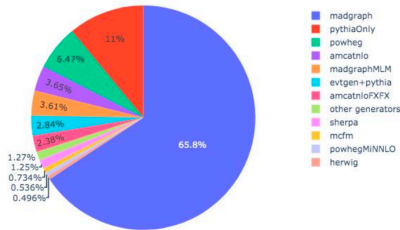
T. Hahn, The Cuba Library – p.20

GENERATORS USAGE IN ATLAS/CMS - 2015/16

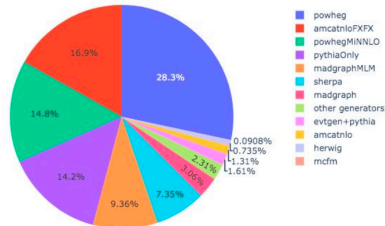
based on Run-2 MC
campaign for 2016 data

CMS

number of samples by generator



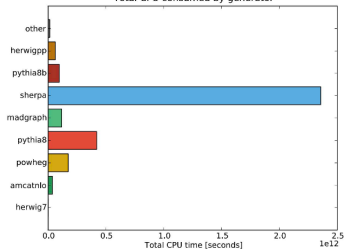
number of events by generator



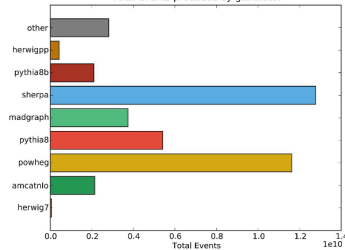
based on Run-2 MC
campaign for 2015 data

ATLAS

Total CPU consumed by generator



Total Events produced by generator



Abstract

Title: Monte Carlo event generators and parton showers

Monte Carlo event generators and parton showers are fundamental tools in modern particle physics research and serve as indispensable components in both theoretical and experimental studies. We introduce basic concepts of Monte Carlo methods and highlight their application to event generation as well as their optimization techniques. An overview of the event generation process is provided, with a focus on combining next-to-leading order hard scattering with parton distribution functions and parton showers using factorization.