Monte Carlo Methods in High Energy Physics

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Lecture 3: MC simulations of HEP processes.

- Motivation.
- Lorentz-invariant phase space (LIPS).
- A general Monte Carlo algorithm for LIPS.
- Multi-branching Monte Carlo algorithms.
- A simple example of MC simulation of a HEP process.

 \Rightarrow http://cern.ch/placzek

Motivation

- In a typical high-energy particle collision there can be many final-state particles (even hundreds!).
- In a theoretical description of particle collision processes one has to deal with complicated multi-dimensional integrals:

 \vartriangleright for n final-state parcicles we have $d=3n-4\;$ dimensional phase space,

e.g. for n = 4: d = 8 – difficult for semi-analytical integration!

(analytical and/or numerical-quadrature)

- Experimental cuts, selection criteria, etc. are usually very complicated too difficult to be dealt with semi-analytical methods. Practically, the only way to account for them in theoretical calculations is through Monte Carlo methods.
- In theoretical description of particle collision processes within the quantum field theory (QED, EW, QCD, SUSY) one often has to deal with multitude of Feynman diagrams of various topologies. These diagrams can have complicated peaking behavior over the phase space.

- Experimental detectors are very complex devices. They need themselves detailed Monte Carlo modeling in order to translate electronic signals into physical observables.
- Full detector simulation programs are usually huge and slow, therefore, they require unweighted ('physical') events in the input (propagating weighted events through such programs would be highly inefficient).
- Therefore, theoretical predictions for particle collision processes should be provided in terms of Monte Carlo Event Generators (MCEG), which directly simulate these processes and can provide unweighted (weight = 1) events.
 Monte Carlo Integrators (MCI), which can provide only weighed events, are usually not sufficient!
- MCEGs are needed at all stages of HEP experiments: preparation, running, data analysis.
- LEP2 experiments have widely used MCEGs for fitting of the Standard Model parameters to experimental data (reweighting methods) – they have probably set up the standards in this area for the future HEP experiments.

Lecture 3: MC simulations of HEP processes



INFN and University of Pavia, 18-22 October 2004

Lorentz-invariant phase space

The cross section for a typical HEP process with n particles in the final state is given by:

$$\sigma_n = \frac{1}{Flux} \int |\mathcal{M}|^2 \, dR_n,$$

where: \mathcal{M} – the matrix element describing the interactions between the particles;

 dR_n – the element of the Lorentz-invariant phase space (LIPS).

► The LIPS is defined as:

$$R_n(P; p_1, p_2, \dots, p_n) = \int \delta^{(4)} \left(P - \sum_{k=1}^n p_k \right) \prod_{k=1}^n \delta(p_k^2 - m_k^2) \Theta(p_k^0) \, d^4 p_k,$$

where: P - the total four-momentum of the n-particle system, p_k , m_k - four-momenta and masses of the final-state particles; $\delta^{(4)} \left(P - \sum_{k=1}^{n} p_k\right)$ - total energy-momentum conservation, $\delta(p_k^2 - m_k^2)$ - on-mass-shell condition for the final-state particles.

▷ On-mass-shell delta functions can be integrated out, giving:

$$\delta(p_k^2 - m_k^2)\Theta(p_k^0) \, d^4 p_k = \frac{d^3 p_k}{2p_k^0} = \frac{|\vec{p}_k|^2}{2p_k^0} \, d|\vec{p}_k| \, d\cos\theta_k \, d\phi_k \, d\phi_$$

 \Rightarrow Number of integration dimensions for n final-state particles: d = 3n - 4!

- \bullet Let's concentrate first on the LIPS (e.g. $\mathcal{M}\simeq$ const.):
- ▷ E. Fermi, Progr. Theoret. Phys. 5 (1950) 570: Non-relativistic and ultra-relativistic approximations to simplify calculations generally too crude for HEP processes.
- \triangleright M. Block, Phys. Rev. **101** (1956) 796: exact analytical integration prohibively complex for $n \ge 4$ particles.
- ▷ G. Kopylov, JEPT 8 (1959) 996: use of the Monte Carlo method to solve the Fermi phase-space problem.
- ▷ P.P. Srivastava and G. Sudarshan, Phys. Rev. **110** (1958) 765: the Lorentz-invariant formulation of the Fermi phase space (as given above) and the recurrence relation:

$$R_n(P; p_1, \dots, p_n) = \int R_{n-1}(P - p_n; p_1, \dots, p_{n-1}) \frac{d^3 p_n}{2p_n^0}.$$



► The above formula can be iterated further:

 \triangleright Let's introduce the following notation:

$$k_i = p_1 + \ldots + p_i, \quad k_i^2 = M_i^2, \quad \mu_i = m_1 + \ldots + m_i;$$

and instert into the recurrence relation the identities:

$$1 = \int dM_{n-1}^2 \,\delta(M_{n-1}^2 - k_{n-1}^2), \quad 1 = \int d^4k_{n-1} \,\delta^{(4)}(P - p_n - k_{n-1}).$$

 \Rightarrow We obtain:

$$\begin{aligned} R_n(M_n^2) &= \int dM_{n-1}^2 \int d^4k_{n-1} \int d^4p_n \, \delta(M_{n-1}^2 - k_{n-1}^2) \, \delta(p_n^2 - m_n^2) \\ &\times \delta^{(4)}(P - p_n - k_{n-1}) \, R_{n-1}(M_{n-1}^2) \\ &= \int dM_{n-1}^2 \, R_2(k_n^2; k_{n-1}^2, p_n^2) \, R_{n-1}(M_{n-1}^2) \\ &= \int dM_{n-1}^2 \, R_2(k_n^2; k_{n-1}^2, p_n^2) \dots \int dM_2^2 \, R_2(k_2^2; p_2^2, p_1^2) \, . \end{aligned}$$

 \rightarrow Pictorially: sequential decay



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 \triangleright The two-particle phase space R_2 can be expressed as follows:

$$R_2(k_i^2; k_{i-1}^2, p_i^2) = \frac{P_i}{4M_i} \int d\Omega_{i-1} = \frac{\sqrt{\lambda(M_i^2, M_{i-1}^2, m_i^2)}}{8M_i^2} \int d\Omega_{i-1} ,$$

where the solid angle Ω_{i-1} describes the orientation of \vec{k}_{i-1} in the rest frame of k_i , and $\lambda(x, y, z) = x^2 + y^2 + z^2 - 2xy - 2xz - 2yz$.

> The limits on the invariant massess are:

$$\mu_{i-1} \le M_{i-1} \le M_i - m_i, \quad i = 3, \dots, n.$$

► Inserting the above in the last expression for the *n*-particle phase space, we obtain: $R_n(M_n^2) = \frac{1}{2M_n} \int_{\mu_{-1}}^{M_n - m_n} dM_{n-1} d\Omega_{n-1} \frac{1}{2} P_n \dots \int_{\mu_2}^{M_3 - m_3} dM_2 d\Omega_2 \frac{1}{2} P_3 \int d\Omega_1 \frac{1}{2} P_2.$

This formula gives the simplest description of the n-particle phase space – it can be used as a basis for Monte Carlo simulations.

 \triangleright We have:

- $\mathbf{n-2}$ invariant masses $M_i,~M_i^2=k_i^2$, defined as masses of intermediate particles;
- 2n 2 angles θ_i , ϕ_i in $\Omega_i = (\cos \theta_i, \phi_i)$, i = 1, ..., n 1. They define the direction $\vec{k}_i = -\vec{p}_{i+1}$ in the rest frame of $\vec{k}_{i+1} = \vec{0}$ of the decay $k_{i+1} \rightarrow p_{i+1} + k_i$.

Splitting relation

Let's derive a more general version of the recurrence relation. Using the identities:

$$\delta^{(4)}(P - k_l - \sum_{i=l+1}^n p_i) = \int d^4k_l \,\delta^{(4)}(P - k_l - \sum_{i=l+1}^n p_i) \,\delta^{(4)}(k_l - \sum_{i=1}^l p_i) \,,$$

$$1 = \int dM_l^2 \,\delta(k_l^2 - M_l^2) \,,$$

we get:

$$R_n(M_n^2) = \int dM_l^2 \int d^4k_l \,\delta(k_l^2 - M_l^2) \int \prod_{i=l+1}^n d^4p_i \,\delta(p_i^2 - m_i^2) \,\delta^{(4)}(P - k_l - \sum_{i=l+1}^n p_i) \\ \times \int \prod_{i=1}^l d^4p_i \,\delta(p_i^2 - m_i^2) \,\delta^{(4)}(k_l - \sum_{i=1}^l p_i) \,,$$

which can be cast in the form of the **splitting relation**:

$$R_{n}(P; p_{1}, \dots, p_{n}) = \int dM_{l}^{2} R_{n-l+1}(P; k_{l}, p_{l+1}, \dots, p_{n}) R_{l}(k_{l}; p_{1}, \dots, p_{l})$$

$$\rightarrow \text{Pictorially:}$$

$$P = R_{n-l+1} P_{l+1} P_$$

The splitting formula can be further iterated to get:

$$R_n(M_n^2) = \frac{1}{2M_n} \int_{\mu_{n-1}}^{M_n - m_n} dM_{n-1} d\Omega_{n-1} \frac{1}{2} P_n \dots \int_{\mu_2}^{M_3 - m_3} dM_2 d\Omega_2 \frac{1}{2} P_3 \int d\Omega_1 \frac{1}{2} P_2,$$

where: $P_i = \frac{1}{2M_i} \sqrt{\lambda(M_i^2, M_{i-1}^2, m_i^2)}, \quad d\Omega_i = d\cos\theta_i \, d\phi_i.$

 \Rightarrow How to calculate/generate this phase space using Monte Carlo techniques?

$$\triangleright$$
 The basic variables: $(M_i, \cos \theta_i, \phi_i)$.

 \rightarrow Since P_i depends rather mildly on M_i and does not depend on $\cos \theta_i$ and ϕ_i , we can absorb it in the MC weight:

$$w_i^P = \frac{1}{2}P_i \,,$$

and generate the variables $(M_i, \cos \theta_i, \phi_i)$ uniformly over their allowed regions.

• Generation of angles

The angles ϕ_i and θ_i can be generated in the frame $k_{i+1} = (M_{i+1}, \vec{0})$ according to: $\phi_i = 2\pi r'_i, \quad \cos \theta_i = 2r''_i - 1, \quad i = 2, \dots, n-1,$ where $r'_i, r''_i \in \mathcal{U}(0, 1)$, i.e. uniformly distributed random numbers over (0, 1), and the orientation of the coordinate-system axes can be chosen arbitrary (this may not be true in general – the matrix element may depend on this orientation, e.g. spin effects).

• Generation of invariant masses

The limits for the invarians masses are:

$$\mu_i \leq M_i \leq M_{i+1} - m_{i+1}, \quad i = 2, \dots, n-1,$$

i.e. they form the (n-2)-dimensional simplex.



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 \triangleright The total volume of the integration domain is:

$$V = \frac{1}{(n-2)!} (M_n - \mu_n)^{n-2} \prod_{i=2}^n (4\pi).$$

It can be included, together with the overall factor $1/(2M_n)$, in the total MC weight:

$$w^{R_n} = \frac{1}{2M_n} \frac{1}{(n-2)!} (M_n - \mu_n)^{n-2} \prod_{i=2}^n (2\pi P_i) .$$

For the MC estimator of R_n and its statistical error for N generated events:

$$\hat{R}_n = \frac{1}{N} \sum_{j=1}^N w_j^{R_n}, \quad \hat{\sigma}(\hat{R}_n) = \frac{1}{\sqrt{N-1}} \sqrt{\frac{1}{N} \sum_{j=1}^N (w_j^{R_n})^2 - (\hat{R}_n)^2}$$

• If the matrix element \mathcal{M} is a mild function of $(M_i, \cos \theta_i, \phi_i)$, it can also be absorbed in the MC event weight:

$$w^{\text{tot}} = w^{R_n} |\mathcal{M}|^2$$

 \Rightarrow If unweighted events are needed, one has to find the maximum weight w_{\max}^{tot} (analytically or with the help a trial MC sample) and apply the rejection method (hit-or-miss Monte Carlo) in the course of the Monte Carlo event generation.

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Construction of the event:

Having generated n-2 invariant masses and 2(n-1) angles, we can construct the event, i.e. calculate the four-momenta p_1, \ldots, p_n of all the particles in any frame. * First, in the frame: $p_1 + p_2 = (M_2, \vec{0})$ we obtain: $p_1^0 = M_2 - p_2^0$, $p_2^0 = (M_2 + m_2 - m_1)/(2M_2),$ $\vec{p}_2 = P_2(\sin\theta_2\cos\phi_2, \sin\theta_2\sin\phi_2, \cos\theta_2), \quad \vec{p}_1 = -\vec{p}_2$ * Then, in a similar way p_3 is constructed in the frame $k_2 + p_3 = (M_3, \vec{0})$, where $k_2 = p_1 + p_2$. The four-momenta p_1 and p_2 are then obtained in this frame by a Lorentz boost along the direction $\vec{k}_2 = -\vec{p}_3$ from the previous frame $k_2 = (M_2, \vec{0})$. * This is continued until the last four-momentum, i.e. p_n , is constructed. The above scenario works well for the processes where the matrix element $\mathcal{M} \approx const.$ However, for many HEP processes this is not true – the matrix element may be a strongly varying function of some of the invariant masses as well as the angles, (e.g. Breit-Wigner

resonances, peripheral collisions, etc.). In such cases, for those invariant masses and

angles one needs to perform importance sampling (or use other MC technique).

 \triangleright A type of an algorithm as preseted above was a basis of the MC program FOWL

by F. James, CERN Computer Program Library, W505 (1970).

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The **splitting relation** can be applied to the n-particle process in many possible ways, which results in various tree diagrams. The number of possible topologically different tree diagrams increases rapidly with n.

Multi-branching MC algorithms: a $2 \to 4$ example

- For 2 → 4 processes we have 2 non-trivial topologies and about 50 permutations.
 ▷ In this case the phase space can be parametrized in terms of 2 invariant masses and 6 angles.
- ▷ From Feynman diagrams one may know possible types of singularities in the invariant masses: 1, 1/s, $1/[(s-M^2)^2+M^2\Gamma^2]$,... and angles: 1, 1/t, $1/t^2$, $1/(t-M^2)$,....



This leads to many branches in the MC algorithm, each representing one tree diagram and one assignment of singularities. The branches are weighted with probabilities, which are estimated analytically or numerically. Distributions in particular branches are generated with the basic MC methods (usually some kind of the importance sampling).

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A. Born approximation:

$$e^+(p_1) + e^-(p_2) \longrightarrow \mu^+(q_1) + \mu^-(q_2)$$

where p_i and q_i denote four-momenta of the corresponding particles.

The matrix element in the Standard Model is given by two basic Feynman diagrams (the Higgs boson contribution is numerically negligible):



▷ Let's consider the process in the centre-of-mass (CMS) frame of the incoming beams:



The differential cross section:

$$\frac{d\sigma}{d\Omega} = \frac{\alpha^2}{4s} \left[W_1(s)(1 + \cos^2 \theta) + W_2(s) \cos \theta \right] ,$$

where: $d\Omega = d\cos\theta \, d\phi$, $\alpha = e^2/4\pi$ is the fine structure constant, and $s = (p_1^0 + p_2^0)^2$ – the CMS energy squared.

The coefficients W_1 and W_2 are given by:

$$W_{1}(s) = 1 + \frac{2(s - M_{Z}^{2})s c_{V}^{2}}{|Z(s)|^{2}} + \frac{s^{2}(c_{V}^{2} + c_{A}^{2})^{2}}{|Z(s)|^{2}}$$
$$W_{2}(s) = \frac{4(s - M_{Z}^{2})s c_{A}^{2}}{|Z(s)|^{2}} + \frac{8s^{2}c_{V}^{2}c_{A}^{2}}{|Z(s)|^{2}}$$

where:

$$Z(s) = s - M_Z^2 + iM_Z\Gamma_Z,$$

$$c_A = \frac{1}{4\sin\theta_W\cos\theta_W}, \quad c_V = -c_A(4\sin^2\theta_W - 1), \quad \cos\theta_W = \frac{M_W}{M_Z},$$

with M_Z , Γ_Z – the Z-boson mass and width, resp., M_W – the W-boson mass. \triangleright Note that for the pure QED process (γ -exchange only):

$$W_1^{\gamma}(s) = 1, \qquad W_2^{\gamma}(s) = 0.$$

For the current vaules of particle masses, widths and other parameters see the Review of Particle Physics, PDG 2004, http://pdg.lbl.gov/

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Monte Carlo simulation

► The total cross section:

$$\sigma = \int_0^{2\pi} d\phi \int_{-1}^1 d\cos\theta \, \frac{d^2\sigma}{d\phi \, d\cos\theta}$$

 \triangleright Let:

$$\rho(\cos\theta,\phi) \equiv \frac{d^2\sigma}{d\phi\,d\cos\theta},$$

and the function $\tilde{\rho}(\cos\theta, \phi)$ be some approximation of $\rho(\cos\theta, \phi)$; $\tilde{\sigma} = \int d\phi d \cos\theta \tilde{\rho}$. \triangleright Then we can write:

$$\begin{split} \sigma &= \int_{0}^{2\pi} d\phi \int_{-1}^{1} d\cos\theta \,\rho(\cos\theta,\phi) = \int_{0}^{2\pi} d\phi \int_{-1}^{1} d\cos\theta \,\tilde{\rho}(\cos\theta,\phi) \,\frac{\rho(\cos\theta,\phi)}{\tilde{\rho}(\cos\theta,\phi)} \\ &= \tilde{\sigma} \int_{0}^{2\pi} d\phi \int_{-1}^{1} d\cos\theta \,\frac{\tilde{\rho}(\cos\theta,\phi)}{\tilde{\sigma}} \,w(\cos\theta,\phi) = \tilde{\sigma} \,E_{\tilde{\rho}}(w) = \tilde{\sigma} \cdot \langle w \rangle_{\tilde{\rho}}, \\ \text{where the event weight:} \quad w(\cos\theta,\phi) \equiv \frac{\rho(\cos\theta,\phi)}{\tilde{\rho}(\cos\theta,\phi)} \,. \end{split}$$

The Monte Carlo estimators of the expectation value and its standard deviation:

$$\langle w \rangle_{\rm MC} = \frac{1}{n} \sum_{i=1}^{n} w_i, \qquad s_{\rm MC} = \frac{1}{\sqrt{n(n-1)}} \sqrt{\sum_{i=1}^{n} w_i^2 - \frac{1}{n} \left(\sum_{i=1}^{n} w_i\right)^2},$$

The value of the total cross section computed with the Monte Carlo method is:

$$\sigma_{\rm MC} = \tilde{\sigma} \cdot \langle w \rangle_{\rm MC} \ \pm \ \tilde{\sigma} \cdot s_{\rm MC} \,.$$

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B. Single photon initial-state radiation (ISR) in the leading-log (LL) approximation:

$$e^+(p_1) + e^-(p_2) \longrightarrow \mu^+(q_1) + \mu^-(q_2) + \gamma(k)$$

 \triangleright The Feynman diagrams for the real single-photon ISR in the Standard Model:



> Appropriate virtual QED corrections have to be included in order to get finite predictions.

ln the collinear approximation, where $k = (1 - z)p_{1(2)}$, the total cross section reads:

$$\sigma = \int_0^1 dz \, \Phi(z) \, \sigma_0(zs) \,,$$

where $\sigma_0(zs)$ is the Born-level cross section taken at the reduces CMS energy, and $\Phi(z) = \delta(z) \left[1 + \beta \left(\frac{3}{2} + 2 \ln \epsilon \right) \right] + \beta \frac{1 + z^2}{1 - z} \Theta(1 - z - \epsilon), \quad \beta = \frac{\alpha}{\pi} \ln \frac{s}{m_e^2},$ where ϵ is the soft-hard photon separator (a photon is hard if $z < 1 - \epsilon$). \triangleright The function Φ satisfies the condition: $\int_0^1 dz \, \Phi(z) = 1$, i.e. can be treated as a probability density function (pdf).

Monte Carlo simulation

The total cross section:

$$\sigma = \int_0^1 dz \,\Phi(z) \int_0^{2\pi} d\phi \int_{-1}^1 d\cos\theta \,\rho(z,\cos\theta,\phi) \,.$$

If ρ depends weakly on z (below the Z peak), we can approximate it by $\tilde{\rho}(\cos\theta, \phi)$ as in the Born-level case. Then, the cross section becomes:

$$\sigma = \tilde{\sigma} \int_0^1 dz \, \Phi(z) \int_0^{2\pi} d\phi \int_{-1}^1 d\cos\theta \, \frac{\tilde{\rho}(\cos\theta,\phi)}{\tilde{\sigma}} \, w(z,\cos\theta,\phi) = \tilde{\sigma} \cdot \langle w \rangle \,,$$

where the weight: $w(z, \cos \theta, \phi) = \rho(z, \cos \theta, \phi) / \tilde{\rho}(\cos \theta, \phi).$

- ▷ The angles (θ, ϕ) are generated according to $\tilde{\rho}(\cos \theta, \phi)$, as at the Born level. → How to generate *z*?
- Dash The function Φ can be expressed in the following form:

$$\Phi(z) = p_S S(z) + p_H H(z); \qquad p_S, \, p_H \ge 0, \, \, p_S + p_H = 1,$$

$$S(z) = p_S^{-1} \,\delta(z) \left[1 + \beta \left(\frac{3}{2} + 2\ln \epsilon \right) \right], \quad H(z) = p_H^{-1} \beta \, \frac{1 + z^2}{1 - z} \,\Theta(1 - z - \epsilon),$$

where S and H satisfy the condition: $\int_0^1 dz \, S(z) = \int_0^1 dz \, H(z) = 1$.

• Generation of z

- \triangleright We can apply the branching (composition) method:
 - * Generate $r \in \mathcal{U}(0,1)$.
 - * If $r \leq p_S = 1 + \beta \left(\frac{3}{2} + 2 \ln \epsilon \right)$, choose $z = 1 \rightarrow \text{soft photon}$.
 - * If $r > p_S$, generate z according to $H(z) \rightarrow$ hard photon.

Warning: ϵ cannot be too small, because p_S has to be non-negative!

ightarrow How to generate z according to H(z)?

Use e.g. importance sampling with the approximate distribution:

$$\tilde{H}(z) \propto rac{1}{1-z} \Theta(1-z-\epsilon)$$

and apply the rejection method for the weight: $w = H(z)/\tilde{H}(z)$.

 $arphi ilde{H}(z)$ can be efficiently generated using the inverse transform method.

• Kinematics

▷ Having the variables $(z, \cos \theta, \phi)$, we can construct the four-momenta of the muons.

* We start from the effective frame CMS':
$$q_1' + q_2' = (\sqrt{s', 0}), \ s' = zs$$
, where:

$$q_1' = (\frac{\sqrt{s'}}{2}, q \sin \theta \cos \phi, q \sin \theta \sin \phi, q \cos \theta), \ q_2' = (q_1'^0, -\vec{q_1'}); \ q = \sqrt{\frac{s'}{4} - m_{\mu}^2}.$$

* Then, we perform a Lorentz boost CMS' \rightarrow CMS: $p_1 + p_2 = (\sqrt{s}, \vec{0})$ along:

$$q_1 + q_2 = p_1 + p_2 - k = \frac{\sqrt{s}}{2}(1 + z, 0, 0, \pm [1 - z]),$$

with the 3rd axis direction chosen randomly: $r \in \mathcal{U}(0,1)$: if r < 0.5: +, else: -.

Summary

- Monte Carlo event generators are indispensable tools in HEP experiments necessary at all their stages: preparation, running, data analysis.
- Multi-particle phase space can be dealt in practice only with the Monte Carlo techniques.
- Using the recurrence relation or the splitting relation for the Lorentz-invariant phase space, one can construct a general MC algorithm for particle collision processes.
- Matrix elements of multi-particle processes may contain various types of singularities. They are usually treated with multi-branching algorithms, where each branch accounts for one assignment of the singularities.
- After generating random points according to desired distributions, given by appropriate differenctial cross sections, one can construct events, i.e. calculate all particles four-momenta in an arbitrary Lorentz frame.
- A good MC algorithm should allow not only for integration (i.e. provide weighted events) but also for efficient generation of unweighted events.