#### Introduction to Monte Carlos

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#### Outline

- Part I Basics
  - Introduction
  - Monte Carlo techniques
- Part II Perturbative physics
  - Hard scattering
  - Parton showers
- Part III Non–perturbative physics
  - Hadronization
  - Hadronic decays
  - Comparison to data

Thanks to my colleagues

# Frank Krauss, Leif Lönnblad, Steve Mrenna, Peter Richardson, Mike Seymour, Torbjörn Sjöstrand.

# Introduction

#### We want to understand

 $\mathscr{L}_{int} \longleftrightarrow Final \mbox{ states }.$ 

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#### Can you spot the Higgs?





### Experiment and Simulation



#### Monte Carlo Event Generators

- Complex final states in full detail (jets).
- Arbitrary observables and cuts from final states.
- Studies of new physics models.
- Rates and topologies of final states.
- Background studies.
- Detector Design.
- Detector Performance Studies (Acceptance).
- Obvious for calculation of observables on the quantum level

 $|A|^2 \longrightarrow$  Probability.

















#### Divide and conquer

#### Partonic cross section from Feynman diagrams

$$d\sigma = d\sigma_{hard} dP(partons \rightarrow hadrons)$$

Note, that

$$\int dP(\text{partons} \to \text{hadrons}) = 1 \; ,$$

- $\sigma$  remains unchanged
- introduce realistic fluctuations into distributions.

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Simulation steps governed by different scales  $\rightarrow$  separation into ( $Q_0 \approx 1 \text{ GeV} > \Lambda_{\text{OCD}}$ )

$$\begin{split} dP(\text{partons} \to \text{hadrons}) &= dP(\text{resonance decays}) & [\Gamma > Q_0] \\ &\times dP(\text{parton shower}) & [\text{TeV} \to Q_0] \\ &\times dP(\text{hadronisation}) & [\sim Q_0] \\ &\times dP(\text{hadronic decays}) & [O(\text{MeV})] \end{split}$$

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Quite complicated integration.

Monte Carlo is the only choice.

# **Monte Carlo Methods**

Introduction to the most important MC sampling (= integration) techniques.

- 1. Hit and miss.
- 2. Simple MC integration.
- 3. (Some) methods of variance reduction.
- 4. Multichannel.

Probability density:

$$dP = f(x) dx$$

is probability to find value *x*.



*Probability*  $\sim$  *Area* 

Probability density:

$$dP = f(x) dx$$

is probability to find value *x*.

$$F(x) = \int_{x_0}^x f(x) \, dx$$

is called *probability distribution*.



 $Probability \sim Area$ 

Hit and miss method:

- ► throw *N* random points (*x*, *y*) into region.
- ▶ Count hits N<sub>hit</sub>,
  i.e. whenever y < f(x).</li>

Then

$$I \approx V \frac{N_{\rm hit}}{N}.$$

approaches 1 again in our example.

*Example:* 
$$f(x) = \cos(x)$$
.



Every accepted value of *x* can be considered an event in this picture. As f(x) is the 'histogram' of *x*, it seems obvious that the *x* values are distributed as f(x) from this picture.

This method is used in many event generators. However, it is not sufficient as such.

- Can handle any density f(x), however wild and unknown it is.
- f(x) should be bounded from above.
- ► Sampling will be very *inefficient* whenever Var(*f*) is large.

Improvements go under the name variance reduction as they improve the error of the crude MC at the same time. Mean value theorem of integration:

$$I = \int_{x_0}^{x_1} f(x) dx$$
  
=  $(x_1 - x_0) \langle f(x) \rangle$   
 $\approx (x_1 - x_0) \frac{1}{N} \sum_{i=1}^N f(x_i)$ 

(Riemann integral).

Sum doesn't depend on ordering  $\longrightarrow$  randomize  $x_i$ .

Yields a flat distribution of events  $x_i$ , but weighted with *weight*  $f(x_i) (\rightarrow \text{unweighting})$ .

## Inverting the Integral

- ► Probability density *f*(*x*). Not necessarily normalized.
- Integral F(x) known,
- $\blacktriangleright P(x < x_s) = F(x_s) \ .$
- Probability = 'area', distributed evenly,

$$\int_{x_0}^x dP = r \cdot \text{area}$$



Sample *x* according to f(x) with

$$x = F^{-1} \Big[ F(x_0) + r \big( F(x_1) - F(x_0) \big) \Big] \,.$$

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Optimal method, but we need to know

- The integral  $F(x) = \int f(x) dx$ ,
- It's inverse  $F^{-1}(y)$ .

That's rarely the case for real problems.

But very powerful in combination with other techniques.

Error on Crude MC  $\sigma_{MC} = \sigma / \sqrt{N}$ .

 $\implies$  Reduce error by reducing variance of integrand.

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Idea: Divide out the singular structure.

$$I = \int f \, \mathrm{d}V = \int \frac{f}{p} p \, \mathrm{d}V \approx \left\langle \frac{f}{p} \right\rangle \pm \sqrt{\frac{\langle f^2/p^2 \rangle - \langle f/p \rangle^2}{N}}$$

where we have chosen  $\int p \, dV = 1$  for convenience.

*Note:* need to sample flat in p dV, so we better know  $\int p dV$  and it's inverse.

### Importance sampling — better example



#### Importance sampling — better example







$$\frac{1}{2\sqrt{x}}$$

with some wiggles,

$$p(x) = 1 - 8x + 40x^2 - 64x^3 + 32x^4$$

i.e. we want to integrate

$$f(x) = \frac{p(x)}{2\sqrt{x}} \, .$$



#### Importance sampling — better example

- Crude MC gives result in reasonable 'time'.
- Error a bit unstable.
- Event generation with maximum weight w<sub>max</sub> = 20. (that's arbitrary.)
- ▶ hit/miss/events with (w > w<sub>max</sub>) = 36566/963434/617 with 1M generated events.



### Importance sampling — example

#### Want events:

use hit+mass variant here:

- Choose new random number r
- w = f(x) in this case.
- ▶ if r < w/w<sub>max</sub> then "hit".
- MC efficiency = hit/N.
- Efficiency for MC events only 3.7%.
- Note the wiggly histogram.


Now importance sampling, i.e. divide out  $1/2\sqrt{x}$ .

$$\int_{0}^{1} \frac{p(x)}{2\sqrt{x}} dx = \int_{0}^{1} \left( \frac{p(x)}{2\sqrt{x}} \middle/ \frac{1}{2\sqrt{x}} \right) \frac{dx}{2\sqrt{x}}$$
$$= \int_{0}^{1} p(x) d\sqrt{x}$$
$$= \int_{0}^{1} p(x(\rho)) d\rho$$
$$= \int_{0}^{1} 1 - 8\rho^{2} + 40\rho^{4} - 64\rho^{6} + 32\rho^{8} d\rho$$

so,

$$\rho = \sqrt{x}, \qquad d\rho = \frac{dx}{2\sqrt{x}}$$

*x* sampled with *inverting the integral* from flat random numbers  $\rho$ ,  $x = \rho^2$ .

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Events generated with  $w_{max} = 1$ , as  $p(x) \le 1$ , no guesswork needed here! Now, we get 74.6% MC efficiency.



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 $\ldots$  as opposed to 3.7%.

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Crude MC vs Importance sampling.

 $100 \times$  more events needed to reach same accuracy.

Typical problem:

► f(s) has multiple peaks (× wiggles from ME).



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- ► f(s) has multiple peaks (× wiggles from ME).
- Usually have some idea of the peak structure.
- Encode this in sum of sample functions g<sub>i</sub>(s) with weights α<sub>i</sub>, Σ<sub>i</sub> α<sub>i</sub> = 1.

$$g(s) = \sum_i \alpha_i g_i(s) \; .$$



Now rewrite

$$\int_{s_0}^{s_1} f(s) ds = \int_{s_0}^{s_1} \frac{f(s)}{g(s)} g(s) ds$$
$$= \int_{s_0}^{s_1} \frac{f(s)}{g(s)} \sum_i \alpha_i g_i(s) ds$$
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Now  $g_i(s) ds = d\rho_i$  (inverting the integral).

Select the distribution  $g_i(s)$  you'd like to sample next event from acc to weights  $\alpha_i$ .

 $\alpha_i$  can be optimized after a number of trials.

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Works quite well:



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## Some Remarks/Real Life MC

- Didn't discuss random number generators. Please make sure to use 'good' random numbers.
- Didn't discuss stratified sampling (VEGAS).
   Sample where variance is biggest.
   (not necessarily where PS is most populated).
- ► Only discussed one-dimensional case here. N-particle PS has 3N 4 dimensions...
- Didn't discuss tools geared towards this, like RAMBO (generates flat N particles PS).
- ► generalisation straightforward, particularly MCError  $\sim \frac{1}{\sqrt{N}}$ , compare eg Trapezium rule Error  $\sim \frac{1}{N^{2/D}}$ .
- Many important techniques covered here in detail! Should be good starting point.

# Hard Scattering

## Hard scattering



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## Matrix elements

 Perturbation theory/Feynman diagrams give us (fairly accurate) final states for a few number of legs (O(1)).



- OK for very inclusive observables.
- Starting point for further simulation.
- ▶ Want exclusive final state at the LHC (*O*(100)).
- Want arbitrary cuts.
- $\rightarrow$  use Monte Carlo methods.

Where do we get (LO)  $|M|^2$  from?

- ► Most/important simple processes (SM) are 'built in'.
- ► Calculate yourself (≤ 3 particles in final state).
- Matrix element generators:
  - MadGraph/MadEvent.
  - Comix/AMEGIC (part of Sherpa).
  - HELAC/PHEGAS.
  - Whizard.
  - CalcHEP/CompHEP.

generate code or event files that can be further processed.

•  $\rightarrow$  FeynRules interface to ME generators.

From Matrix element, we calculate

$$\boldsymbol{\sigma} = \int f_i(x_1, \mu^2) f_j(x_2, \mu^2) \frac{1}{F} \overline{\boldsymbol{\Sigma}} |M|^2 \qquad dx_1 dx_2 d\Phi_n ,$$

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now,

$$\frac{1}{F} dx_1 dx_2 d\Phi_n = J(\vec{x}) \prod_{i=1}^{3n-2} dx_i \qquad \left( d\Phi_n = (2\pi)^4 \delta^{(4)}(\dots) \prod_{i=1}^n \frac{d^3 \vec{p}}{(2\pi)^3 2E_i} \right)$$

such that

$$\begin{split} \sigma &= \int g(\vec{x}) \, \mathrm{d}^{3n-2} \vec{x} , \qquad \left( g(\vec{x}) = J(\vec{x}) f_i f_j \overline{\sum} |M|^2 \Theta(\mathrm{cuts}) \right) \\ &= \frac{1}{N} \sum_{i=1}^N \frac{g(\vec{x}_i)}{p(\vec{x}_i)} = \frac{1}{N} \sum_{i=1}^N w_i . \end{split}$$

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We generate events  $\vec{x}_i$  with weights  $w_i$ .

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where  $w_{\text{max}}$  has to be chosen sensibly.  $\rightarrow$  reweighting, when  $\max(w_i) = \bar{w}_{\text{max}} > w_{\text{max}}$ , as

$$P_i = \frac{w_i}{\bar{w}_{\max}} = \frac{w_i}{w_{\max}} \cdot \frac{w_{\max}}{\bar{w}_{\max}} ,$$

*i.e.* reject events with probability  $(w_{\text{max}}/\bar{w}_{\text{max}})$  afterwards. (can be ignored when #(events with  $w_i > \bar{w}_{\text{max}})$  small.)

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Generate events with same frequency as in nature!

Some comments:

Use techniques from above to generate events efficiently. Goal: small variance in w<sub>i</sub> distribution! Some comments:

- Use techniques from above to generate events efficiently. Goal: small variance in w<sub>i</sub> distribution!
- ► Clear from above: efficient generation closely tied to knowledge of *f*(*x*<sub>i</sub>), *i.e.* the matrix element's propagator structure.

 $\rightarrow$  build phase space generator already while generating ME's automatically.

## **Parton Showers**

#### Hard matrix element



#### Hard matrix element $\rightarrow$ parton showers



► Know short distance (short time) fluctuations from matrix element/Feynman diagrams: *Q* ~ few GeV to *O*(TeV).

► Measure hadronic final states, long distance effects, Q<sub>0</sub> ~ 1GeV.

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Dominated by large logs, terms

$$\alpha_S^n \log^{2n} \frac{Q}{Q_0} \sim 1$$
.

Generated from emissions *ordered* in *Q*.
Quarks and gluons in final state, pointlike.

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Dominated by large logs, terms

$$\alpha_S^n \log^{2n} \frac{Q}{Q_0} \sim 1$$
.

Generated from emissions *ordered* in *Q*. Soft and/or collinear emissions.

# $e^+e^-$ annihilation

Good starting point:  $e^+e^- \rightarrow q\bar{q}g$ :

Final state momenta in one plane (orientation usually averaged). Write momenta in terms of

$$x_{i} = \frac{2p_{i} \cdot q}{Q^{2}} \quad (i = 1, 2, 3) ,$$
  

$$0 \le x_{i} \le 1 , x_{1} + x_{2} + x_{3} = 2 ,$$
  

$$q = (Q, 0, 0, 0) ,$$
  

$$Q \equiv E_{cm} .$$

Fig: momentum configuration of  $q, \bar{q}$  and g for given point  $(x_1, x_2), \bar{q}$  direction fixed.

$$(x_1, x_2) = (x_q, x_{\bar{q}})$$
 –plane:



Differential cross section:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}x_1\mathrm{d}x_2} = \sigma_0 \frac{C_F \alpha_S}{2\pi} \frac{x_1 + x_2}{(1 - x_1)(1 - x_2)}$$

Collinear singularities:  $x_1 \rightarrow 1$  or  $x_2 \rightarrow 1$ . Soft singularity:  $x_1, x_2 \rightarrow 1$ .





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Collinear singularities:  $x_1 \rightarrow 1$  or  $x_2 \rightarrow 1$ . Soft singularity:  $x_1, x_2 \rightarrow 1$ .

Rewrite in terms of  $x_3$  and  $\theta = \angle(q,g)$ :

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\cos\theta\mathrm{d}x_3} = \sigma_0 \frac{C_F \alpha_S}{2\pi} \left[ \frac{2}{\sin^2\theta} \frac{1 + (1 - x_3)^2}{x_3} - x_3 \right]$$

Singular as  $\theta \to 0$  and  $x_3 \to 0$ .





## $e^+e^-$ annihilation

Can separate into two jets as

$$\frac{2d\cos\theta}{\sin^2\theta} = \frac{d\cos\theta}{1-\cos\theta} + \frac{d\cos\theta}{1+\cos\theta}$$
$$= \frac{d\cos\theta}{1-\cos\theta} + \frac{d\cos\bar{\theta}}{1-\cos\bar{\theta}}$$
$$\approx \frac{d\theta^2}{\theta^2} + \frac{d\bar{\theta}^2}{\bar{\theta}^2}$$

#### e<sup>+</sup>e<sup>-</sup> annihilation

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So, we rewrite  $d\sigma$  in collinear limit as

$$d\sigma = \sigma_0 \sum_{\text{jets}} \frac{d\theta^2}{\theta^2} \frac{\alpha_S}{2\pi} C_F \frac{1 + (1 - z)^2}{z^2} dz$$

#### e<sup>+</sup>e<sup>-</sup> annihilation

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$$egin{aligned} \mathrm{d}\sigma &= \sigma_0 \sum_{\mathrm{jets}} rac{\mathrm{d} heta^2}{ heta^2} rac{lpha_S}{2\pi} C_F rac{1+(1-z)^2}{z^2} \mathrm{d}z \ &= \sigma_0 \sum_{\mathrm{jets}} rac{\mathrm{d} heta^2}{ heta^2} rac{lpha_S}{2\pi} P(z) \mathrm{d}z \end{aligned}$$

with DGLAP splitting function P(z).

#### Universal DGLAP splitting kernels for collinear limit:

$$\mathrm{d}\sigma = \sigma_0 \sum_{\mathrm{jets}} \frac{\mathrm{d}\theta^2}{\theta^2} \frac{\alpha_S}{2\pi} P(z) \mathrm{d}z$$











$$P_{q \rightarrow gq}(z) = C_F \frac{1 + (1-z)^2}{z}$$



 $P_{q \to qq}(z) = T_R(1 - 2z(1 - z))$ 

Universal DGLAP splitting kernels for collinear limit:

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Note: Other variables may equally well characterize the collinear limit:

$$\frac{\mathrm{d}\theta^2}{\theta^2} \sim \frac{\mathrm{d}Q^2}{Q^2} \sim \frac{\mathrm{d}p_{\perp}^2}{p_{\perp}^2} \sim \frac{\mathrm{d}\tilde{q}^2}{\tilde{q}^2} \sim \frac{\mathrm{d}t}{t}$$

whenever  $Q^2, p_{\perp}^2, t \rightarrow 0$  means "collinear".

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whenever  $Q^2, p_{\perp}^2, t \to 0$  means "collinear".

- $\theta$ : HERWIG
- $Q^2$ : PYTHIA  $\leq$  6.3, old Sherpa.
- ▶  $p_{\perp}$ : PYTHIA ≥ 6.4, ARIADNE, Catani–Seymour showers in HERWIG++ and SHERPA.
- ▶ q̃: Herwig++.

Need to introduce resolution  $t_0$ , e.g. a cutoff in  $p_{\perp}$ . Prevent us from the singularity at  $\theta \rightarrow 0$ .

Emissions below  $t_0$  are unresolvable.

Finite result due to virtual corrections:

unresolvable + virtual emissions are included in Sudakov form factor via unitarity (see below!).

Starting point: factorisation in collinear limit, single emission.

$$\sigma_{2+1}(t_0) = \sigma_2(t_0) \int_{t_0}^t \frac{\mathrm{d}t'}{t'} \int_{z_-}^{z_+} \mathrm{d}z \frac{\alpha_S}{2\pi} \hat{P}(z) = \sigma_2(t_0) \int_{t_0}^t \mathrm{d}t \, W(t) \; .$$

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Simple example: Multiple photon emissions, strongly ordered in *t*. We want

for any number of emissions.

We used

$$\int_{t_0}^t dt_1 \dots \int_{t_0}^{t_{n-1}} dt_n \ W(t_1) \dots W(t_n) = \frac{1}{n!} \left( \int_{t_0}^t dt \ W(t) \right)^n \, .$$

Easily generalized to n emissions  $\phi_{i}$  by induction. *i.e.* 

$$W_{2+n} = \frac{2^n}{n!} \left( \int_{t_0}^t \mathrm{d}t \, W(t) \right)^n$$

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So, in total we get

$$\sigma_{>2}(t_0) = \sigma_2(t_0) \sum_{k=1}^{\infty} \frac{2^k}{k!} \left( \int_{t_0}^t dt \, W(t) \right)^k = \sigma_2(t_0) \left( e^{2 \int_{t_0}^t dt \, W(t)} - 1 \right)$$

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$$\begin{aligned} \sigma_{>2}(t_0) &= \sigma_2(t_0) \sum_{k=1}^{\infty} \frac{2^k}{k!} \left( \int_{t_0}^t dt \, W(t) \right)^k = \sigma_2(t_0) \left( e^{2\int_{t_0}^t dt \, W(t)} - 1 \right) \\ &= \sigma_2(t_0) \left( \frac{1}{\Delta^2(t_0, t)} - 1 \right) \end{aligned}$$

Sudakov Form Factor

$$\Delta(t_0,t) = \exp\left[-\int_{t_0}^t \mathrm{d}t \, W(t)\right]$$

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Sudakov Form Factor in QCD

$$\Delta(t_0,t) = \exp\left[-\int_{t_0}^t \mathrm{d}t \, W(t)\right] = \exp\left[-\int_{t_0}^t \frac{\mathrm{d}t}{t} \int_{z_-}^{z_+} \frac{\alpha_S(z,t)}{2\pi} \hat{P}(z,t) \mathrm{d}z\right]$$

#### Sudakov form factor

Note that

$$\begin{split} \sigma_{\mathrm{all}} &= \sigma_2 + \sigma_{>2} = \sigma_2 + \sigma_2 \left( \frac{1}{\Delta^2(t_0, t)} - 1 \right) \ , \\ &\Rightarrow \Delta^2(t_0, t) = \frac{\sigma_2}{\sigma_{\mathrm{all}}} \ . \end{split}$$

Two jet rate  $= \Delta^2 = P^2$  (No emission in the range  $t \to t_0$ ).

Sudakov form factor = No emission probability .

Often  $\Delta(t_0, t) \equiv \Delta(t)$ .

- ▶ Hard scale *t*, typically CM energy or  $p_{\perp}$  of hard process.
- ► Resolution t<sub>0</sub>, two partons are resolved as two entities if inv mass or relative p<sub>⊥</sub> above t<sub>0</sub>.
- ▶ *P*<sup>2</sup> (not *P*), as we have two legs that evolve independently.