

# Simulations in High Energy Physics

H. Jung (DESY)

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Oxford advanced dictionary: simulate = pretend to be

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Oxford advanced dictionary: simulate = pretend to be  
or  
Film Studios....



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  - Detector response
  - Particle decays
  - ep, e<sup>-</sup>e<sup>+</sup>, pp interactions
  - Economy
  - Life

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  - Economy
  - Life
- Simulation: How-to?

# Application in Economy

What is monte carlo simulation? montecarlo analysis?

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# Application in Risk Management

# Application in Risk Management

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 Summary: This document introduces the concept of Monte Carlo methods by ... a simple example (the determination of pi) using a Monte Carlo simulation!  
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 A brief online text book on Monte Carlo Methods by Paul Coddington, Syracuse  
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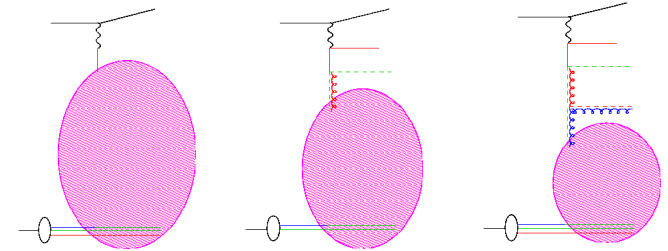
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# Where is the problem ?



QPM process  
total x-section

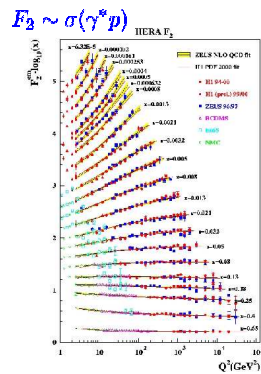
BGF process  
heavy quarks (charm & bottom)  
2-jet  $\mathcal{O}(\alpha_s)$

process  
3-jet  $\mathcal{O}(\alpha_s^2)$

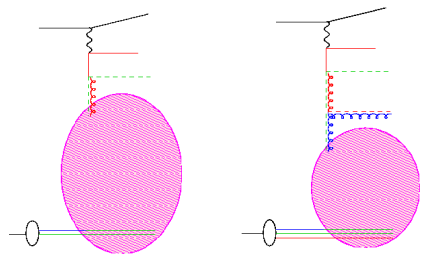
H. Jung, Simulations in HEP, Summerstudent Lecture, 2007

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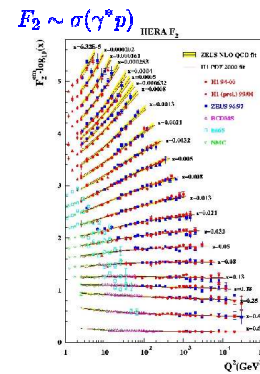
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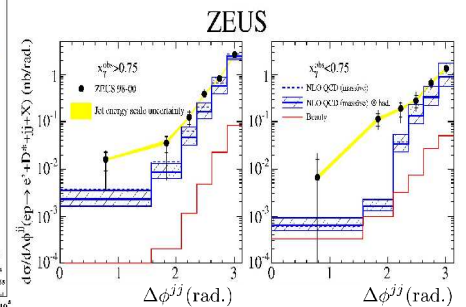
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# Where is the problem: hadronic final state



QPM process  
total x-section



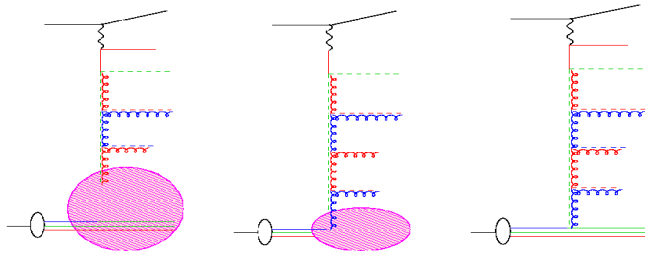
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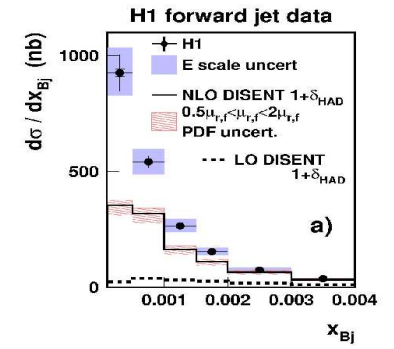
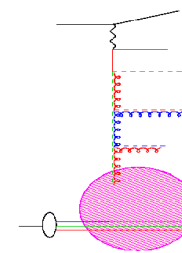
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## Where is the problem: hadronic final state



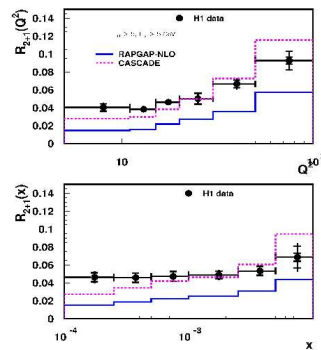
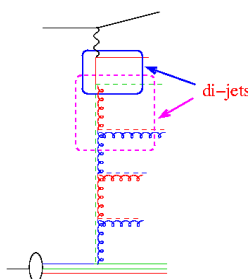
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interesting to go closer to outgoing proton remnant  
forward jets !!!

## Where is the problem: hadronic final state



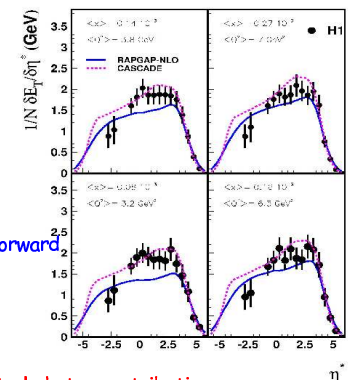
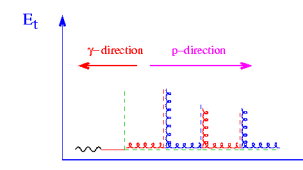
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## Hadronic final state: Di-jet rates



- (2+remnant) jets in DIS for  $Q^2 > 5 \text{ GeV}^2$ ,  $p_{T,jets} > 5 \text{ GeV}$
- $\mathcal{O}(\alpha_s)$  processes not enough  
→ need  $\mathcal{O}(\alpha_s^2)$  or resolved virtual photon contributions  
→ or something new ???

## Hadronic final state: Energy flow



- $E_t$  flow in DIS at small  $x$  and forward angle ( $p$ -direction):  
→  $\mathcal{O}(\alpha_s)$  processes not enough
- need  $\mathcal{O}(\alpha_s^2)$  or resolved virtual photon contributions
- or something new ???

# How to simulate these processes ?

## Monte Carlo method

- Monte Carlo method
  - **refers** to any procedure that makes use of random numbers
  - **uses** probability statistics to solve the problem
- Monte Carlo methods are used in:
  - Simulation of natural phenomena
  - Simulation of experimental apparatus
  - Numerical analysis
- Random number:

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**No such thing as a single random number**

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- Random number:

one of them is 3

**No such thing as a single random number**

A sequence of random numbers is a set of numbers that have nothing to do with the other numbers in a sequence

## Going out to Monte Carlo



- Obtain true Random Numbers from Casino in Monte Carlo
- Puhhh... Going out every night ...

## Random Numbers

- In a uniform distribution of random numbers in  $[0,1]$  every number has the same chance of showing up
- Note that 0.000000001 is just as likely as 0.5

To obtain random numbers:

- Use some chaotic system like roulette, lotto, 6-49, ...
- Use a process, inherently random, like radioactive decay
- Tables of a few million truly random numbers exist ....  
(.....until a few years ago.....)

**BUT** not enough for most applications

- Hooking up a random machine to a computer is **NOT toooooo good**, as it leads to irreproducible results, making debugging difficult....
- **Develop Pseudo Random Number generators !!!!**

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Pseudo means: Oxford Advanced Dict.: **False**  
 Quasi means: Oxford Advanced Dict.: **almost**  
**BUT** here the meaning is different

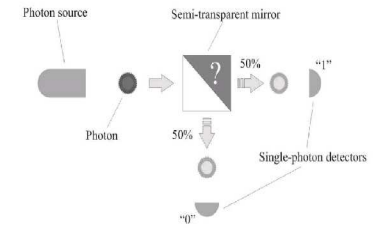
## Quasi Random Numbers

- mathematical randomness is not attainable in computer generated random numbers
- more important: assure that the "random" sequence has the necessary properties to produce a desired result ... ( hmmm !!! )
- examples:
  - in multidimensional integration, each multi-dim point is considered independently of the others, and the order in which they appear plays no role !
  - degree of fluctuations about uniformity: in many cases a "super-uniform" distribution is more desirable than a truly random distribution with uniform probability density !
- use of Quasi Random Numbers might lead to faster convergence of the integration .... but needs to be checked carefully ...

Important in  
Monte Carlo integrations

## True Random Numbers

- Random numbers from classical physics: coin tossing
  - evolution of such a system can be predicted, once the initial condition is known... however it is a chaotic process ... extremely sensitive to initial conditions.
- Truly Random numbers used for
  - Cryptography
  - Confidentiality
  - Authentication
  - Scientific Calculation
  - Lotteries and gambling
  - do not allow to increase chance of winning by having a bias .... too bad
- Random numbers from quantum physics: intrinsic random photons on a semi-transparent mirror
  - Available and tested in MC generator by a summer student
  - Generator is however very slow...



## Pseudo Random Numbers

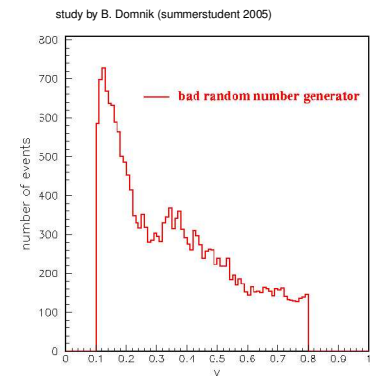
### Pseudo Random Numbers

- are a sequence of numbers generated by a computer algorithm, usually uniform in the range [0,1]
- more precisely: algo's generate integers between 0 and M, and then  $r_n = I_n / M$
- A very early example: Middles Square (John van Neumann, 1946):
  - generate a sequence, start with a number of 10 digits, square it, then take the middle 10 digits from the answer, as the next number etc.:
  - $5772156649^2 = 33317792380594909291$
  - Hmmm, sequence is not random, since each number is determined from the previous, but it appears to be random
- this algorithm has problems .....
  - BUT a more complex algo does not necessarily lead to better random sequences ....
  - Better us an algo that is well understood

## Random Number generators

Compare random number generators with physics process

- $\gamma$  spectrum of electron
  - observe peaks
  - coming from physics ?

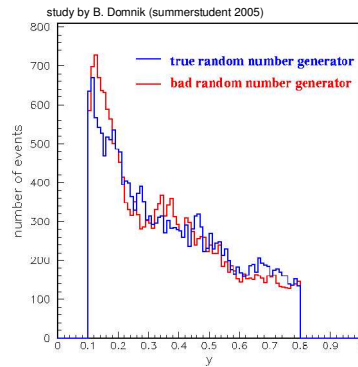




## Random Number generators

Compare random number generators with physics process

- $\gamma$  spectrum of electron
  - observe peaks
  - coming from physics ?
- BUT coming from bad random number generator



From now on assume:  
we have good random number generator

## Simulating Radioactive Decay

- radioactive decay is a truly random process
- $dN = -N \alpha dt$  i.e.  $N = N_0 e^{-\alpha t}$
- probability of decay is **constant** ... independent of the age of the nuclei: probability that nucleus undergoes radioactive decay in time  $\Delta t$  is  $p$ :  
 $p = \alpha \Delta t$  (for  $\alpha \Delta t \ll 1$ )
- **Problem:**  
consider a system initially having  $N_0$  unstable nuclei.  
How does the number of parent nuclei,  $N$ , change with time ?
- **Algorithm:**

```

LOOP from t=0 to t, step  $\Delta t$ 
  LOOP over each remaining parent nucleus
    Decide if nucleus decays:
    IF ( random # <  $\alpha \Delta t$  ) then
      reduce number of parents by 1
    ENDIF
  END LOOP over nuclei
  Plot or record  $N$  vrs  $t$ 
END LOOP over time
END
    
```

## The first simulation: radioactive decay

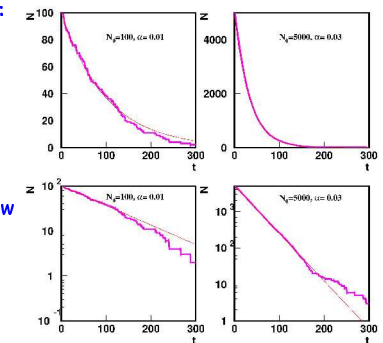
- implement algo into a small program
- show results after 3000 sec for:
  - $N_0 = 100, \alpha = 0.01 \text{ s}^{-1}$   
 $\Delta t = 1 \text{ s}$
  - $N_0 = 5000, \alpha = 0.03 \text{ s}^{-1}$   
 $\Delta t = 1 \text{ s}$

```

• algo:
  alphas = 0.01
  N01 = 100
  deltat = 1
  do i=1,3000
    it = it + 1
    do j = 1, N01
      x = RN1
      fr = deltat*alpha
      if(x.lt.fr) then
c   reduce number of parents N01
        N01 = N01 - 1
      endif
c   fill for each time it number N01
      call hfill(400,real(it+0.3),0,1.) !
    enddo
  enddo
    
```

## The first simulation: radioactive decay

- implement algo into a small program
- show results after 3000 sec for:
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  - $N_0 = 5000, \alpha = 0.03 \text{ s}^{-1}$   
 $\Delta t = 1 \text{ s}$
- MC experiment does not exactly reproduce theory ....
- results from MC experiment show statistical fluctuations ...
- .....as expected .....



## Monte Carlo technique: basics

- Law of large numbers

chose  $N$  numbers  $u_i$  randomly, with probability density uniform in  $[a,b]$ , evaluate  $f(u_i)$  for each  $u_i$  :

$$\frac{1}{N} \sum_{i=1}^N f(u_i) \rightarrow \frac{1}{b-a} \int_a^b f(u) du$$

for large enough  $N$  Monte Carlo estimate of integral converges to correct answer.

- Convergence

is given with a certain probability ...

**THIS is a mathematically serious and precise statement !!!!**

## Expectation values and variance

- Expectation value (defined as the average or mean value of function  $f$ ):

$$E[f] = \int f(u) dG(u) = \left( \frac{1}{b-a} \int_a^b f(u) du \right) = \frac{1}{N} \sum_{i=1}^N f(u_i)$$

for uniformly distributed  $u$  in  $[a,b]$  then  $dG(u) = du/(b-a)$

- rules for expectation values:

$$E[cx + y] = cE[x] + E[y]$$

- Variance

$$V[f] = \int (f - E[f])^2 dG = \left( \frac{1}{b-a} \int_a^b (f(u) - E[f])^2 du \right)$$

- rules for variance:

if  $x,y$  uncorrelated:  $V[cx + y] = c^2V[x] + V[y]$

if  $x,y$  correlated

$$V[cx + y] = c^2V[x] + V[y] + 2cE[(y - E[y])(x - E[x])]$$

## Central Limit Theorem

- Central Limit Theorem

for large  $N$  the sum of independent random variables is always normally (Gaussian) distributed:

$$f(x) = \frac{1}{s\sqrt{2\pi}} \exp \left[ -\frac{(x-a)^2}{2s^2} \right]$$

- example: take sum of uniformly distributed random numbers:

$$\begin{aligned} R_n &= \sum_{i=1}^n R_i \\ E[R_1] &= \int u du = 1/2, \\ V[R_1] &= \int (u - 1/2)^2 du = 1/12 \\ E[R_n] &= n/2 \\ V[R_n] &= n/12 \end{aligned}$$

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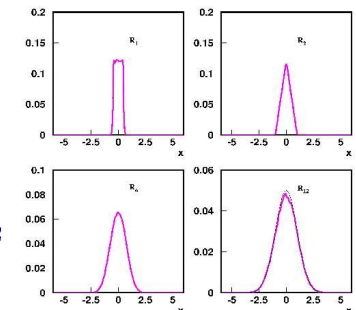
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- for Gaussian with mean=0 and variance=1, take for  $n=12$ :

$$N(0,1) \rightarrow \frac{R_n - n/2}{n/12}$$



## Resume: Monte Carlo technique

- Law of large numbers

$$\frac{1}{N} \sum_{i=1}^N f(u_i) \rightarrow \frac{1}{b-a} \int_a^b f(u) du$$

MC estimate converges to true integral

- Central limit theorem

MC estimate is asymptotically normally distributed  
it approaches a Gaussian density

$$\sigma = \frac{\sqrt{V[f]}}{\sqrt{N}} \sim \frac{1}{\sqrt{N}}$$

with effective variance  $V(f)$

→ to decrease  $\sigma$ , either reduce  $V(f)$  or increase  $N$

- advantages for n-dimensional integral ...  
i.e. phase space integrals  $2 \rightarrow n$  processes  
is where other approaches tend to fail

## Monte Carlo: Buffons Needle - Hit & Miss

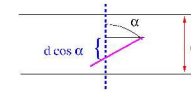
- Buffons needle (Buffon 1777)  
pattern of parallel lines with distance  $d$ ,  
randomly throw needle with length  $d$  onto stripes,  
count hit, when needle crosses strip count miss, if not
- probability for hit is:

$$\frac{d \cos(\alpha)}{d} = \cos(\alpha)$$

all angles are equally likely:

$$\frac{\int_0^{\pi/2} \cos(\alpha) d\alpha}{\pi/2} = \frac{2}{\pi}$$

<http://www.angelfire.com/wa/hurben/buffh.htm>



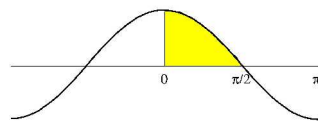
```
loop over ntrials
x=RN(1) * d
alpha = RN(2) * 3.1415 * 2
y = d * abs(cos(alpha))
if ((x+y).gt. d) nhit = nhit + 1
endloop
write ' pi = ', 2*ntrials/nhit
```

trials	$\pi$	error
100	2.9850	0.2374
1000	3.2733	0.0749
10000	3.1645	0.0237
100000	3.1483	0.0075
1000000	3.1401	0.0024
10000000	3.1422	0.0008

## Buffons Needle: Crude Monte Carlo

- Buffons needle (Buffon 1777) is essentially integration of

$$\int_0^{\pi/2} \cos(\alpha) d\alpha$$



- apply Law of large numbers:

$$\frac{1}{N} \sum_{i=1}^N f(u_i) \rightarrow \frac{1}{b-a} \int_a^b f(u) du$$

- compare Hit & Miss with Integration

- 1st example of true Monte Carlo experiment
- equivalence of integration and MC event generation

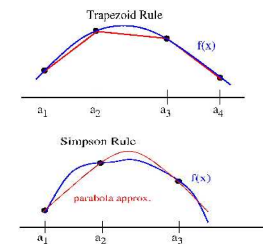
trials	$\pi$ (hit&miss)	$\pi$ (integral)
100	3.27869	3.12265
1000	3.36700	3.11833
10000	3.14218	3.15129
100000	3.13087	3.13416
1000000	3.14127	3.14337
10000000	3.14154	3.14168
100000000	3.12174	3.14156

## Integration: Monte Carlo versus others

One dimensional quadrature

$$I = \int f(x) dx = \sum_{i=1}^n w_i f(x_i)$$

- Monte Carlo: Hit & Miss  
 $w=1$  and  $x_i$  chosen randomly
- Trapezoidal Rule:  
approximate integral in sub-interval  
by area of trapezoid below (above) curve
- Simpson quadrature  
approximate by parabola
- Gauss quadrature  
approximate by higher order polynomial



method	err (1d)	error
MC	$n^{-1/2}$	$n^{-1/2}$
Trapez	$n^{-2}$	$n^{-2/d}$
Simpson	$n^{-4}$	$n^{-4/d}$
Gauss	$n^{-2m+1}$	$n^{-(2m-1)/d}$

## MC method: advantage of hit & miss

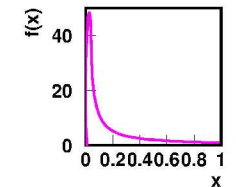
- integration  $\rightarrow$  weighting events
  - large fluctuations from large weights
  - weights also to errors applied
  - difficult to apply further hadronization
- real events all have weight = 1 !!!
- Hit & Miss method:

MC for function  $f(x)$ :  
 get random number:  
 $R1$  in  $(0,1)$  and  $R2$  in  $(0,1)$   
 calculate  $x = R1$   
 reject event if:  $f_x < f_{max} R2$

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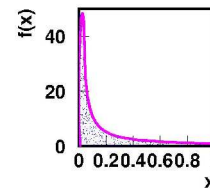
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## MC method: advantage of hit & miss

- integration  $\rightarrow$  weighting events
  - large fluctuations from large weights
  - weights also to errors applied
  - difficult to apply further hadronization
- real events all have weight = 1 !!!
- Hit & Miss method:

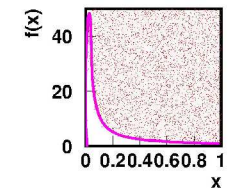
MC for function  $f(x)$ :  
 get random number:  
 $R1$  in  $(0,1)$  and  $R2$  in  $(0,1)$   
 calculate  $x = R1$   
 reject event if:  $f_x < f_{max} R2$



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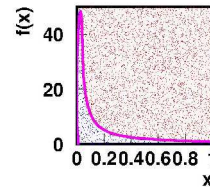
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## MC method: do even better ...

- Importance sampling

MC for function  $f(x)$   
 approximate  $f(x) \sim g(x)$   
 with  $g(x) > f(x)$  simple and integrable  
 generate  $x$  according to  $g(x)$ :

$$\int_{x_{min}}^x g(x') dx' = R1 \int_{x_{min}}^{x_{max}} g(x') dx'$$

example:  $f(x) = 1/x^{0.7}$

$$g(x) = 1/x$$

$$x = x_{min} \cdot \left( \frac{x_{max}}{x_{min}} \right)^{R1}$$

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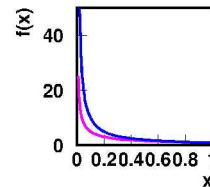
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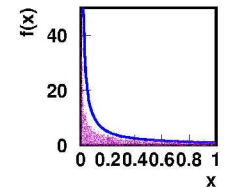
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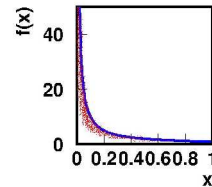
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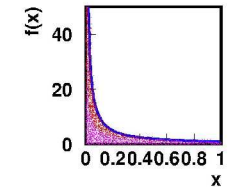
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reject event if:  $f(x) < g(x) R2$



WOW !!! very efficient even for peaked  $f(x)$

## Importance Sampling

### MC calculations most efficient for small weight fluctuations:

$$f(x)dx \rightarrow f(x) dG(x)/g(x)$$

- choose point according to  $g(x)$  instead of uniformly
- $f$  is divided by  $g(x) = dG(x)/dx$
- generate  $x$  according to:

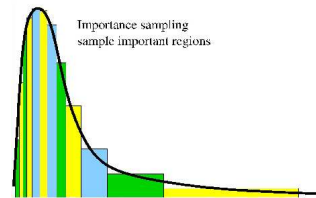
$$R \int_a^b g(x') dx' = \int_a^x g(x') dx'$$

- relevant variance is now  $V(f/g)$ :

small if  $g(x) \sim f(x)$

- how-to get  $g(x)$

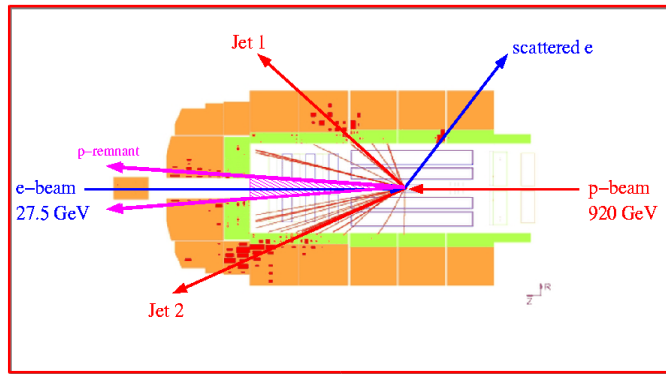
- $g(x)$  is probability:  $g(x) > 0$  and  $\int dG(x) = 1$
- integral  $\int dG(x)$  is known analytically
- $G(x)$  can be inverted (solved for  $x$ )
- $f(x)/g(x)$  is nearly constant, so that  $V(f/g)$  is small compared to  $V(f)$



## Applications in High Energy Physics

- Simulation of detector response
- Apply MC method to  $e^+e^-$
- what about hadronization
- what about QCD radiation
- going even further: initial state radiation
- how-to do a DIS Monte Carlo event generator
- some examples

## MC event: hadron and detector level



$$\sqrt{s} \sim 318 \text{ GeV} \rightarrow x \sim 7 \cdot 10^{-6} \text{ at } Q^2 = 4 \text{ GeV}^2$$

## From experiment to measurement

take data

run MC generator

detailed detector simulation

compare detector level response: data with MC

define visible x-section in kinematic variables  
calculate factor  $C_{corr}$  to correct from detector to hadron level

$$\frac{d\sigma_{had}^{data}}{dx} = \frac{d\sigma_{det}^{data}}{dx} C_{corr} \text{ with } C_{corr} = \frac{d\sigma_{had}^{MC}}{dx} / \frac{d\sigma_{det}^{MC}}{dx}$$

visible x-section on hadron level

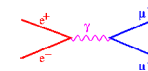
**All measurements rely on proper MC's !!!**

## MC generators - different applications ...

- calculate x-section of various processes  $\rightarrow$  complicated integrals
- multi-differential in any variable
- MC simulation of detector response
  - input: hadron level events - output: detector level events
  - Calorimeter ADC hits
  - Tracker hits
  - need knowledge of particle passage through matter, x-section ...
  - need knowledge of actual detector
  - x-section on parton level
- multipurpose MC event generators:
  - x-section on parton level
  - including multi-parton (initial & final state) radiation
  - remnant treatment (proton remnant, electron remnant)
  - hadronisation/fragmentation (more than simple fragmentation functions...)
- fixed order parton level ..... theorists like it
  - integration of multidimensional phase space

## Constructing a MC for $e^+e^-$ : the simple case

process:  $e^+e^- \rightarrow \mu^+\mu^-$



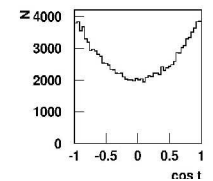
$$\frac{d\sigma}{d\cos\theta d\phi} = \frac{\alpha_{em}^2}{4s} (1 + \cos^2\theta)$$

goal: generate 4-momenta of  $\mu^+$ 's,  
need cm energy  $s$ ,  $\cos\theta$ ,  $\phi$

random number  $R1(0,1)$   $\phi = 2\pi R1$   
random number  $R2(0,1)$   $\cos\theta = -1 + 2R2$

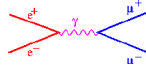
for every  $R1, R2$  use weight with  $\frac{d\sigma}{d\cos\theta d\phi}$   
repeat many times

after 100000 events



## Constructing a MC for $e^+e^-$ : the simple case

- process:  $e^+e^- \rightarrow \mu^+ \mu^-$

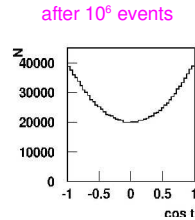


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random number  $R1(0,1) \phi = 2\pi R1$   
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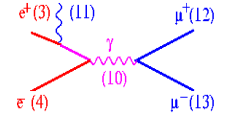
- for every  $R1, R2$  use weight with  $\frac{d\sigma}{d\cos\theta d\phi}$
- repeat many times



## Example event: $e^+e^- \rightarrow \mu^+ \mu^-$

- example from PYTHIA: Event listing

I	particle/jet	KS	KP	orig	p_x	p_y	p_z	E	m
1	le+	21	-11	0	0.000	0.000	30.000	30.000	0.001
2	le-	21	11	0	0.000	0.000	-30.000	30.000	0.001
3	le+	21	-11	1	0.000	0.000	30.000	30.000	0.000
4	le-	21	11	2	0.000	0.000	-30.000	30.000	0.000
5	le+	21	-11	3	0.143	0.040	26.460	26.460	0.000
6	le-	21	11	4	0.000	0.000	-29.998	29.998	0.000
7	l20:	21	23	0	0.143	0.040	-3.539	56.458	56.347
8	lmu-	21	13	7	-9.510	1.741	24.722	26.546	0.106
9	lmu+	21	-13	7	9.653	-1.700	-28.261	29.913	0.106
10	(20)	11	23	7	0.143	0.040	-3.539	56.458	56.347
11	gamma	1	22	3	-0.143	-0.040	3.539	3.542	0.000
12	mu-	1	13	8	-9.510	1.741	24.722	26.546	0.106
13	mu+	1	-13	9	9.653	-1.700	-28.261	29.913	0.106
sum:					0.00	0.000	0.000	60.000	60.000

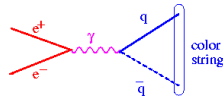


- technicalities/advantages
  - can work in any frame
  - Lorentz-boost 4-vectors back and forth
  - can calculate any kinematic variable
  - history of event process

## Constructing a MC for $e^+e^- \rightarrow q\bar{q}$

- process  $e^+e^- \rightarrow q\bar{q}$

$$\frac{d\sigma}{d\cos\theta d\phi} = \frac{\alpha_{em}^2}{4s} (1 + \cos^2\theta)$$



- generate scattering as for  $e^+e^- \rightarrow \mu^+ \mu^-$
- BUT** what about fragmentation/hadronization ???
- use concept of local parton-hadron duality

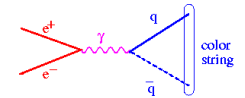
### Different approaches to fragmentation/hadronization:

- independent fragmentation
- string fragmentation (Lund Model)
- cluster fragmentation (HERWIG model)

## Constructing a MC for $e^+e^- \rightarrow q\bar{q}$

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$$\frac{d\sigma}{d\cos\theta d\phi} = \frac{\alpha_{em}^2}{4s} (1 + \cos^2\theta)$$



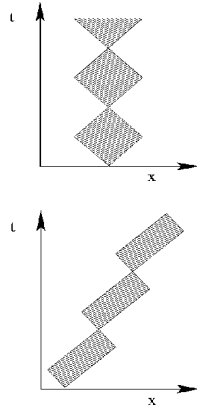
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linear confinement potential:  $V(r) \sim -1/r + \kappa r$   
 with  $\kappa \sim 1 \text{ GeV/fm}$   
 qq connected via color flux tube of transverse size of hadrons ( $\sim 1 \text{ fm}$ )  
 color tube: uniform along its length → linearly rising potential  
 → **Lund string fragmentation**



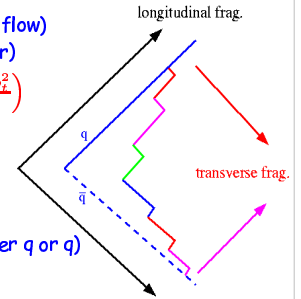
## Lund string fragmentation

- in a color neutral qq-pair, a color force is created in between
- color lines of the force are concentrated in a narrow tube connecting q and q-bar, with a string tension of:  $\kappa \sim 1 \text{ GeV/fm} \sim 0.2 \text{ GeV}^2$
- as q and q-bar are moving apart in qq rest frame, they are de-accelerated by string tension, accelerated back etc ... (periodic oscillation)
- viewed in a moving system, the string is boosted



## Fragmentation in the String Model

- hadronization: iterative process
- string breaks in qq pairs (still respecting color flow)
- select transverse motion with  $m = m_{qq}$  (and flavor)
 
$$P \sim \exp\left(-\frac{\pi m_{qq}^2}{\chi}\right) = \exp\left(-\frac{\pi m_q^2}{\chi}\right) \exp\left(-\frac{\pi p_T^2}{\chi}\right)$$
- suppression of heavy quark production
 
$$u : d : s : c \sim 1 : 1 : 1 : 0.37 : 10^{-10}$$
 actually leave it as a free parameter
- longitudinal fragmentation
 symmetric fragmentation function (from either q or q-bar)
 
$$f(z) \sim z^{-1}(1-z)^a \exp(-b m^2/z)$$
 harder spectrum for heavy quarks
- start from q or q-bar
- repeat until cutoff is reached
- heavy use of random numbers and importance sampling method



## Hadronization: particle masses and decays

- particle masses
  - taken from PDG, where known, otherwise from constituent masses
- particle widths
  - in hard scattering production process short lived particles ( $\rho, \Delta$ ) have nominal mass, without mass broadening
  - in hadronization use Breit-Wigner:

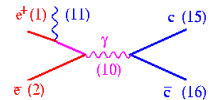
$$P(m)dm \propto \frac{1}{(m - m_0)^2 + \Gamma^2/4}$$

- lifetimes
  - related to widths ... but for practical purpose separated
  - $P(\tau)d\tau \sim \exp(-\tau/\tau_0) d\tau$
  - calculate new vertex position  $v' = v + \tau p/m$
- decays
  - taken from PDG, where known
  - assume momentum distribution given by phase space only
  - exceptions, like  $\omega, \phi \rightarrow \pi^+ \pi^- \pi^0$ , or  $D \rightarrow K\pi$ ,  $D^* \rightarrow K\pi\pi$  and some semileptonic decays use matrix elements

## Example event $e^+e^- \rightarrow qq$

- example from PYTHIA Monte Carlo generator including hadronization

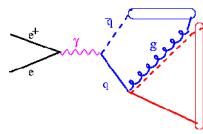
I	particle/jet	KS	KP	orig	p_x	p_y	p_z	E	m	
1	le+	21	-11	0	0.000	0.000	30.000	30.000	0.001	
2	le-	21	11	0	0.000	0.000	-30.000	30.000	0.001	
-----										
5	le+	21	-11	3	0.018	0.040	0.702	0.703	0.000	
6	le-	21	11	4	0.000	0.000	-29.998	29.998	0.000	
-----										
10	(D)	11	23	7	0.018	0.040	-29.297	30.701	9.180	
11	gamma	1	22	1	-0.018	-0.040	29.298	29.298	0.000	
15	(c)	A	12	4	10	-1.950	-3.529	-19.752	20.215	1.500
16	(cbar)	V	11	-4	10	1.967	3.569	-9.545	10.486	1.500
-----										
17	(string)	11	92	15	0.018	0.040	-29.297	30.701	9.180	
18	(D)	11	421	17	-0.455	-1.495	-9.002	9.325	1.865	
19	(omega)	11	223	17	-0.300	-0.076	-3.228	3.338	0.793	
20	pi+	1	211	17	-0.168	-0.172	-0.861	0.904	0.140	
21	(rho-)	11	-213	17	-0.114	-0.513	-4.992	5.106	0.932	
22	(omega)	11	223	17	-0.173	0.118	-2.022	2.180	0.789	
23	pi+	1	211	17	0.226	0.925	-2.593	2.766	0.140	
24	(D*+)	11	-413	17	1.001	1.253	-6.599	7.082	2.010	
25	e+	1	-11	18	-0.191	0.241	-1.261	1.297	0.001	
26	nu_e	1	12	18	-0.154	-0.789	-4.174	4.250	0.000	
-----										
53	pi-	1	-211	47	0.318	-0.061	-1.293	1.340	0.140	
-----										
sum:					0.000	0.000	0.000	60.000	60.000	



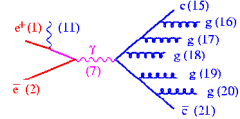
- apply fragmentation directly to parton
- all covered by hadronization .... soft
- where is QCD ???

## Doing things better: $e^+e^- \rightarrow q\bar{q}g$

- process  $e^+e^- \rightarrow q\bar{q}g$
- full matrix element calculation
- watch out color flow !!!
- gluons act as kicks on strings



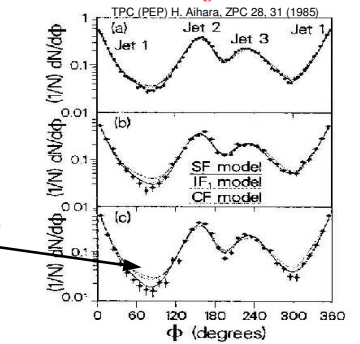
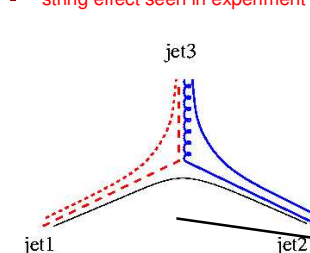
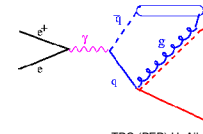
I	particle/jet	KS	KP	orig	p_x	p_y	p_z	E	m	
1	le+	21	-11	0	0.000	0.000	30.000	30.000	0.001	
2	le-	21	11	0	0.000	0.000	-30.000	30.000	0.001	
-----										
5	le+	21	-11	1	0.000	0.000	29.699	29.699	0.000	
6	le-	21	11	2	-1.319	-1.236	-26.950	27.011	0.000	
7	l201	21	23	0	-1.319	-1.236	2.748	56.710	56.614	
8	lc+	21	4	7	-15.986	16.072	18.293	29.167	1.500	
9	lcb-	21	-4	7	14.667	-17.308	-15.545	27.542	1.500	
-----										
11	gamma	1	22	2	1.320	1.236	-2.744	3.286	0.000	
15	(c)	A	12	4	-11.291	11.550	13.219	20.926	1.500	
16	(g)	I	12	21	8	-3.992	3.139	4.805	6.991	0.000
17	(g)	I	12	21	8	-0.279	0.951	0.379	1.007	0.000
18	(g)	I	12	21	8	0.122	-0.178	-0.505	0.550	0.000
19	(g)	I	12	21	9	0.128	-0.237	0.146	0.307	0.000
20	(g)	I	12	21	9	-0.093	-0.746	-0.164	0.835	0.000
21	(g)	I	12	21	9	8.331	-6.743	-6.396	12.482	0.000
22	(cbar)	V	11	-4	9	5.754	-8.971	-8.335	13.613	1.500



- more large  $p_T$  emissions
- not all covered by fixed order calculations
- doing much better needed
- parton shower approach

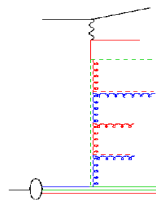
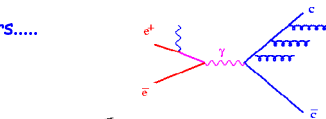
## Glucos in string fragmentation

- process  $e^+e^- \rightarrow q\bar{q}g$
- watch out color flow !!!
- gluons act as kicks on strings
- string effect seen in experiment



## Approximations to higher orders: parton showers

- Approximation to higher orders.....
- fragmentation functions
- parton density functions



- since  $\alpha_s$  is not small, higher orders contributions are important
- Approximations:

**DGLAP** (Dokshitzer, Gribov, Lipatov, Altarelli, Parisi )  
**BFKL** (Balitski, Fadin, Kuraev, Lipatov)  
**CCFM** (Catani, Ciafaloni, Fiorani, Marchesini)

## DGLAP equation

- differential form  $q \frac{\partial}{\partial q} f(x, q) = \int \frac{dz}{z} \frac{\alpha_s}{2\pi} P_+(z) f\left(\frac{x}{z}, q\right)$

- modified differential form using "Sudakov form factor"

$$\Delta_s(q_0, q) = \exp\left(-\bar{\alpha}_s \int \frac{dz}{z} \int_{q_0}^q \frac{dq'}{q'} \tilde{P}(z)\right)$$

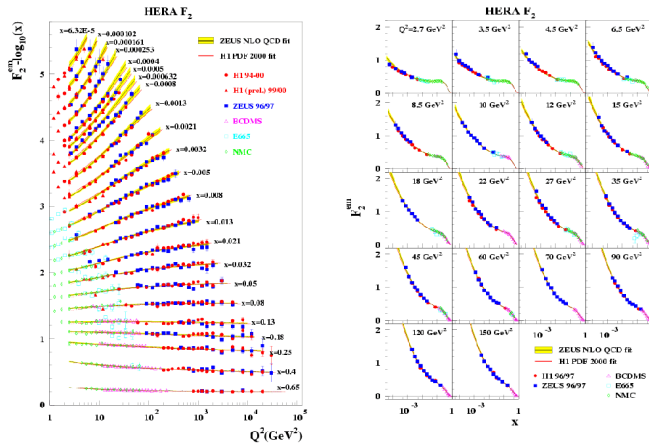
$$q \frac{\partial}{\partial q} \frac{f(x, q)}{\Delta_s(q, q_0)} = \int \frac{dz}{z} \frac{\alpha_s}{2\pi} \frac{\tilde{P}(z)}{\Delta_s(q, q_0)} f\left(\frac{x}{z}, q\right)$$

- integral form

$$f(x, q) = f_0(x, q) \Delta_s(q, q_0) + \int \frac{dz}{z} \int \frac{dq'}{q'} \cdot \Delta_s(q', q_0) \tilde{P}(z) f\left(\frac{x}{z}, q'\right)$$

- no-branching probability form  $q_0$  to  $q$

## Applying DGLAP to DIS data ...



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## Solving DGLAP equations ...

- Different methods to solve integro-differential equations

- brute-force (BF) method (M. Miyama, S. Kumano CPC 94 (1996) 185)

$$\frac{df(x)}{dx} = \frac{f(x)_{m+1} - f(x)_m}{\Delta x_m} \int f(x) dx = \sum f(x)_m \Delta x_m$$

- Laguerre method (S. Kimano J.T. Londergan CPC 69 (1992) 373, and L. Schoeffel Nucl.Instrum.Meth.A423:439-445,1999)
- Mellin transforms (M. Gluck, E.Reyn, A. Vogt Z. Phys. C48 (1990) 471)
- QCDNUM: calculation in a grid in  $x, Q^2$  space (M. Botje Eur.Phys.J. CH (2000) 285-297)
- CTEQ evolution program in  $x, Q^2$  space: <http://www.phys.psu.edu/~cteq/>
- QCDFIT program in  $x, Q^2$  space (C. Pascaud, F. Zomer, LAL preprint LAL/94-02, H1.09/94-404, H1.09/94-376)
- MC method using Markov chains (S. Jodach, M. Skrzypiek hep-ph/0504202)
- Monte Carlo method from iterative procedure
- brute-force method and MC method are best suited for detailed studies of branching processes !!!

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## Solving integral equations

- Integral equation of Fredholm type:  $\phi(x) = f(x) + \lambda \int_a^b K(x,y)\phi(y)dy$
- solve it by iteration (Neumann series):  
 $\phi_0(x) = f(x)$   
 $\phi_1(x) = f(x) + \lambda \int_a^b K(x,y)f(y)dy$   
 $\phi_2(x) = f(x) + \lambda \int_a^b K(x,y_1)f(y_1)dy_1 + \lambda^2 \int_a^b \int_a^b K(x,y_1)K(y_1,y_2)f(y_2)dy_2dy_1$   
 $\phi_n(x) = \sum_{i=0}^n \lambda^i u_i(x)$   
 $u_0(x) = f(x)$   
 $u_1(x) = \int_a^b K(x,y)f(y)dy$   
 $u_n(x) = \int_a^b \int_a^b K(x,y_1)K(y_1,y_2) \dots K(y_{n-1},y_n)f(y_n)dy_2 \dots dy_n$

with the solution:  $\phi(x) = \lim_{n \rightarrow \infty} q_n(x) = \lim_{n \rightarrow \infty} \sum_{i=0}^n \lambda^i u_i(x)$

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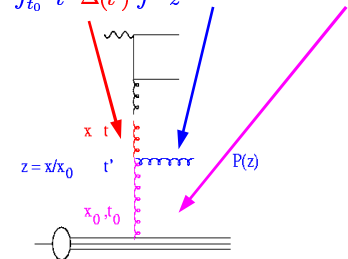
## Solution of DGLAP equation

$$f(x,t) = f(x,t_0)\Delta_s(t) + \int \frac{dz}{z} \int \frac{dt'}{t'} \cdot \frac{\Delta_s(t)}{\Delta_s(t')} \tilde{P}(z) f\left(\frac{x}{z}, t'\right)$$

- solve integral equation via explicit iteration:

$$f_0(x,t) = f(x,t_0)\Delta(t) \quad \begin{array}{l} \text{from } t' \text{ to } t \\ \text{w/o branching} \end{array} \quad \begin{array}{l} \text{branching at } t' \end{array} \quad \begin{array}{l} \text{from } t_0 \text{ to } t' \\ \text{w/o branching} \end{array}$$

$$f_1(x,t) = f(x,t_0)\Delta(t) + \int_{t_0}^t \frac{dt'}{t'} \frac{\Delta(t)}{\Delta(t')} \int \frac{dz}{z} \tilde{P}(z) f(x/z, t_0)\Delta(t')$$



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## DGLAP re-sums leading logs...

$$f(x, t) = f(x, t_0) \Delta_s(t) + \int \frac{dz}{z} \int \frac{dt'}{t'} \cdot \frac{\Delta_s(t)}{\Delta_s(t')} \tilde{P}(z) f\left(\frac{x}{z}, t'\right)$$

- solve integral equation via iteration:

$$f_0(x, t) = f(x, t_0) \Delta(t) \quad \begin{array}{l} \text{from } t' \text{ to } t \\ \text{w/o branching} \end{array} \quad \begin{array}{l} \text{branching at } t' \end{array} \quad \begin{array}{l} \text{from } t_0 \text{ to } t' \\ \text{w/o branching} \end{array}$$

$$f_1(x, t) = f(x, t_0) \Delta(t) + \int_{t_0}^t \frac{dt'}{t'} \frac{\Delta(t)}{\Delta(t')} \int \frac{dz}{z} \tilde{P}(z) f(x/z, t_0) \Delta(t')$$

$$= f(x, t_0) \Delta(t) + \log \frac{t}{t_0} A \otimes \Delta(t) f(x/z, t_0)$$

$$f_2(x, t) = f(x, t_0) \Delta(t) + \log \frac{t}{t_0} A \otimes \Delta(t) f(x/z, t_0) +$$

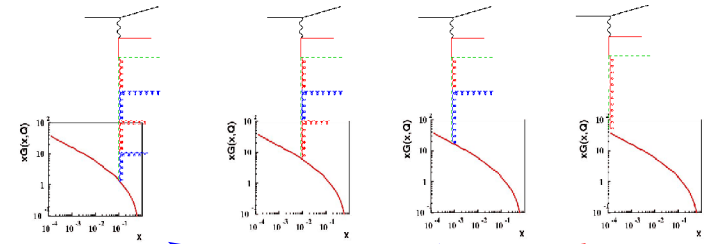
$$\frac{1}{2} \log^2 \frac{t}{t_0} A \otimes A \otimes \Delta(t) f(x/z, t_0)$$

$$f(x, t) = \lim_{n \rightarrow \infty} f_n(x, t) = \lim_{n \rightarrow \infty} \sum_n \frac{1}{n!} \log^n \left( \frac{t}{t_0} \right) A^n \otimes \Delta(t) f(x/z, t_0)$$

**DGLAP re-sums  $\log t$  to all orders !!!!!!!!!!!!!!!!**

## Parton showers to solve DGLAP evolution

- for fixed  $x$  and  $Q^2$  chains with different branchings contribute
- iterative procedure, **spacelike** parton showering



$$f(x, t) = \sum_{k=1}^{\infty} f_k(x_k, t_k) + f_0(x, t_0) \Delta_s(t)$$

## Parton showers for the initial state

**spacelike ( $Q < 0$ ) parton shower evolution**

- starting from hadron (fwd evolution) or from hard scattering (bwd evolution)

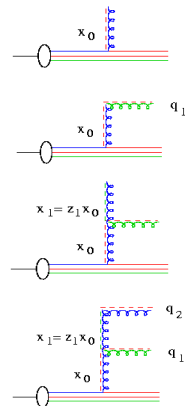
- select  $q_1$  from Sudakov form factor

- select  $z_1$  from splitting function

- select  $q_2$  from Sudakov form factor

- select  $z_2$  from splitting function

- stop evolution if  $q_2 > Q_{\text{hard}}$



## Parton Showers for the final state

**timelike parton shower evolution**

- starting with hard scattering

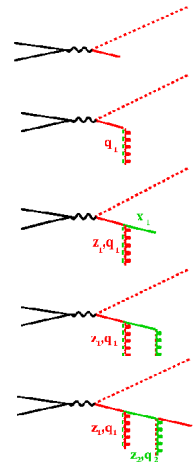
- select  $q_1$  from Sudakov form factor

- select  $z_1$  from splitting function

- select  $q_2$  from Sudakov form factor

- select  $z_2$  from splitting function

- stop evolution if  $q_2 < q_0$



## Parton Shower

- Evolution equation with **Sudakov form factor** recovers exactly evolution equation (with  $\epsilon$  prescription)
- Sudakov form factor** particularly suited form Monte Carlo approach
- Sudakov form factor**
  - gives probability for **no-branching** between  $q_0$  and  $q$
  - sums virtual contributions to all orders (via unitarity)
    - **virtual (parton loop)** and
    - **real (non-resolvable)** parton emissions
- need to specify scale of hard process (matrix element)  $Q \sim p$ ,
- need to specify cutoff scale  $Q_0 \sim 1 \text{ GeV}$

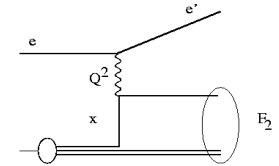
## The DIS process $ep \rightarrow epX$

- cross section

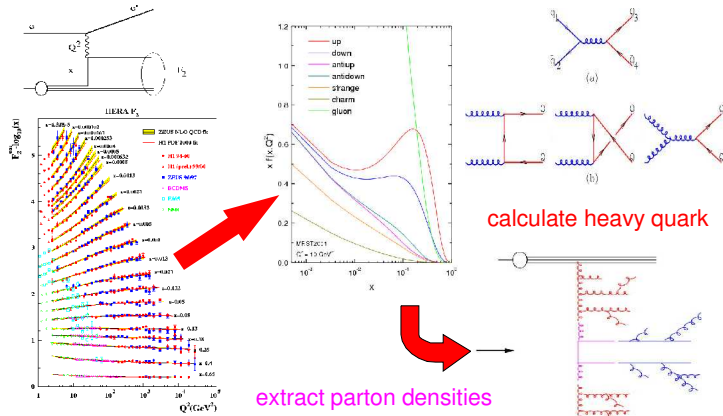
$$\frac{d\sigma(ep \rightarrow e'X)}{dy dQ^2} = \frac{4\pi\alpha^2}{yQ^4} \left( \left(1 - y + \frac{y^2}{2}\right) F_2^p(x, Q^2) - \frac{y^2}{2} F_L^p(x, Q^2) \right)$$

$$\text{with } F_2^p(x, Q^2) = \sum_f e_f^2 (xq_f(x, Q^2) + x\bar{q}_f(x, Q^2))$$

- Exercise:** how to simulate this process ?
  - integration of x-section
  - simulation of events
    - using parton densities and neglect  $F_L$



## From $F_2$ to Heavy Quarks in pp



total x-section,  $F_2$

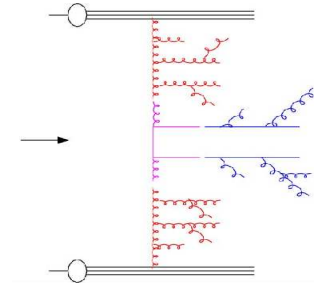
## Heavy Quark production in pp

- x-section

$$\sigma(pp \rightarrow Q\bar{Q}X) = \int \frac{dx_1}{x_1} \frac{dx_2}{x_2} x_1 G(x_1, \bar{q}) x_2 G(x_2, \bar{q}) \times \hat{\sigma}(\hat{s}, \bar{q})$$

- with gluon densities  $xG(x, \bar{q})$
- hard x-section:

$$\frac{d\sigma}{dt} = \frac{1}{64s^2} |M_{ij}|^2$$



## Heavy Quarks in pQCD

### Light Quarks

$$\hat{s} = (p_1 + p_2)^2$$

$$\hat{t} = (p_1 - p_3)^2$$

$$\hat{u} = (p_2 - p_3)^2$$

### Heavy Quarks with

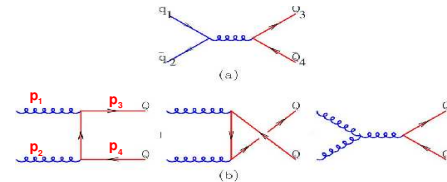
$$\tau_1 = -\frac{\hat{t} - m^2}{\hat{s}}$$

$$\tau_2 = -\frac{\hat{u} - m^2}{\hat{s}}$$

$$\rho = \frac{4m^2}{\hat{s}}$$

Process	$\sum  \mathcal{M} ^2 / g^4$
$q\bar{q} \rightarrow q'\bar{q}'$	$\frac{4}{9} \frac{\hat{t}^2 + \hat{u}^2}{\hat{s}^2}$
$gq \rightarrow q\bar{q}$	$\frac{1}{6} \frac{\hat{t}^2 + \hat{u}^2}{\hat{t}\hat{u}} - \frac{3}{8} \frac{\hat{t}^2 + \hat{u}^2}{\hat{s}^2}$

Ellis, Stirling, Webber  
QCD & Collider physics p348



Process	$\sum  \mathcal{M} ^2 / g^4$
$q\bar{q} \rightarrow Q\bar{Q}$	$\frac{4}{9} (\tau_1^2 + \tau_2^2 + \frac{\rho}{2})$
$gq \rightarrow Q\bar{Q}$	$(\frac{1}{6\tau_1\tau_2} - \frac{3}{8}) (\tau_1^2 + \tau_2^2 + \rho - \frac{\rho^2}{4\tau_1\tau_2})$

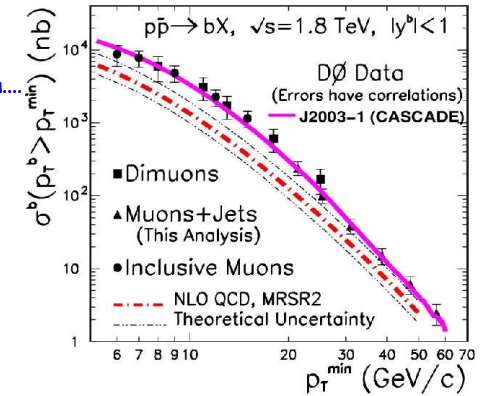
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## bbar at TeVatron

H. Jung, PRD 65, 034015 (2002)  
hep-ph/0110034

- comparison with measurements
- this is what you obtain....



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## Conclusion

- Monte Carlo event generators are needed to calculate multi-parton cross sections
- Monte Carlo method is a well defined procedure
- hadronization is needed to compare with measurements
- parton shower (leading log) approach is needed, hadronization not enough
- MC approach extended from simple e+e- processes to
  - ep processes
  - pp processes
  - and heavy Ion processes
- proper Monte Carlos are essential for any measurement

**Monte Carlo event generators  
contain all our physics  
knowledge !!!!!**

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## List of available MC programs

- HERA Monte Carlo workshop: [www.desy.de/~heramc](http://www.desy.de/~heramc)
- ARIADNE**  
A program for simulation of QCD cascades implementing the color dipole model
- AROMA**  
Heavy quark production in boson-gluon fusion using full electroweak LO cross-sections (with quark masses) in ep collisions, DIS and photoproduction, Parton showers and Lund hadronization gives full events.
- CASCADE**  
is a full hadron level Monte Carlo generator for  $ep$  and  $p\bar{p}$  scattering at small  $x$  build according to the CCFM evolution equation. It is applicable in  $ep$  to photoproduction and DIS, and for heavy quark production as well as inelastic  $J/\psi$ .
- HERWIG**  
General purpose generator for Hadron Emission Reactions With Interfering Gluons; based on matrix elements, parton showers including color coherence within and between jets, and a cluster model for hadronization.
- JETSET**  
The Lund string model for hadronization of parton systems.

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## List of available MC programs

- **LDCMC**  
A program which implements the Linked Dipole Chain (LDC) model for deeply inelastic scattering within the framework of ARIADNE. The LDC model is a reformulation of the CCFM model.
- **LEPTO**  
Deep inelastic lepton-nucleon scattering based on LO electroweak cross sections (incl. lepton polarization), first order QCD matrix elements, parton showers and Lund hadronization giving complete events. Soft color interaction model gives rapidity gap events.
- **PHOJET**  
Multi-particle production in high energy hadron-hadron, photon-hadron, and photon-photon interactions (hadron = proton, antiproton, neutron, or pion).
- **POMPYT**  
Diffractive hard scattering in  $p\bar{p}$ ,  $\gamma$ - $p$  and  $ep$ -collisions, based on pomeron flux and pomeron parton densities (several options included). Also pion exchange is included. Parton showers and Lund hadronization to give complete events.

## List of available MC programs

- **PYTHIA**  
General purpose generator for  $e^+e^-$ ,  $p\bar{p}$  and  $ep$ -interactions, based on LO matrix elements, parton showers and Lund hadronization.
- **RAPGAP**  
A full Monte Carlo suited to describe Deep Inelastic Scattering, including diffractive DIS and LO direct and resolved processes. Also applicable for  $\gamma$ -production and partially for  $p\bar{p}$  scattering.

## General literature

- Many new books are available in DESY library **NEW ... ask at the desk there ...**
- Statistische und numerische Methoden der Datenanalyse  
V. Blobel & E. Lohrmann
- STATISTICAL DATA ANALYSIS. *Glen Cowan.*
- Particle Data Book *S. Eidelman et al., Physics Letters B592, 1 (2004)*  
(<http://pdg.lbl.gov/>)
- Applications of pQCD *R.D. Field Addison-Wesley 1989*
- Collider Physics *V.D. Barger & R.J.N. Phillips Addison-Wesley 1987*
- Deep Inelastic Scattering. *R. Devenish & A. Cooper-Sankar, Oxford 2*
- Handbook of pQCD *G. Sterman et al*
- Quarks and Leptons, *F. Halzen & A.D. Martin, J.Wiley 1984*
- QCD and collider physics *R.K. Ellis & W.J. Stirling & B.R. Webber Cambridge 1996*
- QCD: High energy experiments and theory *G. Dissertori, I. Knowles, M. Schmelling Oxford 2003*

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section on: Mathematical Tools (<http://pdg.lbl.gov/>)
- Michael J. Hurben Buffons Needle  
(<http://www.angelfire.com/wa/hurben/buff.html>)
- J. Woller (Univ. of Nebraska-Lincoln) Basics of Monte Carlo Simulations  
(<http://www.chem.unl.edu/zeng/joy/mdab/mcintro.html>)
- Hardware Random Number Generators:  
A Fast and Compact Quantum Random Number Generator  
(<http://arxiv.org/abs/quant-ph/9912118>)  
Quantum Random Number Generator  
(<http://www.idquantique.com/products/quantis.htm>)  
Hardware random number generator (<http://en.wikipedia.org/wiki/>)
- Monte Carlo Tutorials  
(<http://www.cooper.edu/engineering/chemchem/MMC/tutor.html>)
- History of Monte Carlo Method  
(<http://www.geocities.com/CollegePark/Quad/2435/history.html>)
- Google: search for Monte Carlo Simulations

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<http://www-h1.desy.de/~jung/rapgap.html>  
CASCADE manual  
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Addison-Wesley Publishing Comp. (1987)
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Cambridge University Press (1996)