H. Jung (DESY)

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8

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 Particle decays
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    Simulation: How-to?
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Simulation: what?
    Detector response
    Particle decays
    ep, e<sup>+</sup> e<sup>-</sup>, pp interactions
    Economy
    Life
Simulation: How-to?
    apply Monte Carlo technique:
    solve complicated integrals
```

simulate complicated processes

# Application in Economy

What is monte carlo simulation? montecarlo analysis?

http://www.decisioneering.com/monte-carlo-simulation.html



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#### RISK ANALYSIS OVERVIEW

#### WHAT IS MONTE CARLO SIMULATION?

#### What do we mean by "simulation?"

When we use the word **simulation**, we refer to any analytical method meant to imitate a real-life system, especially when other analyses are too mathematically complex or too difficult to reproduce.

Without the aid of simulation, a spreadsheet model will only reveal a single outcome, generally the most likely or average scenario. Spreadsheet risk analysis uses both a spreadsheet model and simulation to automatically analyze the effect of varying inputs on outputs of the modeled system.

One type of spreadsheet simulation is **Monte Carlo simulation**, which randomly generates values for uncertain variables over and over to simulate a model.

#### How did Monte Carlo simulation get its name?

Monte Carlo simulation was named for Monte Carlo, Monaco, where the primary attractions are casinos containing games of chance. Games of chance such as roulette wheels, dice, and slot machines, exhibit random behavior.

The random behavior in games of chance is similar to how Monte Carlo simulation selects variable values at random to simulate a model. When you roll a die, you know that either a 1, 2, 3, 4, 5, or 6 will come up, but you don't know which for any particular roll. It's the same with the variables that have a known range of values but an uncertain value for any particular time or event (e.g. interest rates, staffing needs, stock prices, inventory, phone calls per minute).

Overview Start

What is Risk?

What is a Model?

Traditional Risk Analysis

Spreadsheet Risk Analysis

Monte Carlo Simulation

Analysis of Results

Benefits of Risk Analysis

Optimization

Time-series Forecasting

### Application in Nuclear Waste ...

Applied Intelligence: The Use of Monte Carlo Simulation...http://www.applied-intelligence.co.uk/Papers/Supercon

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### Applied Intelligence

Business intelligence through knowledge technology

#### Case Study: The Use of Monte Carlo Simulation to Optimise the Supercompaction Process at the Waste Treatment Complex, Sellafield

First published in *Unicom seminar on AI and Optimisation in Process Control* (Heathrow) June 1996

#### **ABSTRACT**

Mathematical modelling and Monte Carlo simulation have been used to model the supercompaction process at WTC, BNFL Sellafield. A better understanding of the process was achieved, and the algorithm initially specified to select drums for compression was found to hav some surprising and undesirable effects. The application of statistical decision theory allowed the development and testing of improved algorithms, which should result in major operational cost savings.

- 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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one of them is 3

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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
- Not 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 generatos !!!!

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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 ... ( hmmmm !!! )
  - 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 ...

### 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<sup>2</sup> = 33317792380594909291
  - Hmmmm, 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

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#### 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 \text{ (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 \Deltat

LOOP over each remaining parent nucleus

Decide if nucleus decays:

IF ( random \# < \alpha \Deltat ) 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 \ s^{-1}
\Delta t = 1s
N_0 = 5000, \ a = 0.03 \ s^{-1}
\Delta t = 1s
```

algo:

```
alpha1 = 0.01
N01 = 100
deltat = 1
do I=1,300
    it = it + 1
    do j = 1, N01
        x = RN1
        fr = deltat*alpha1
        if(x.lt.fr) then

reduce number of parents N01
        N01 = N01 - 1
        endif

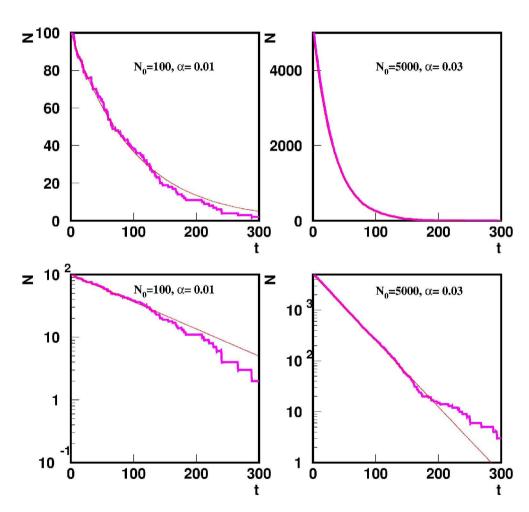
fill for each time it number N01
        call hfill(400,real(it+0.3),0,1.) !
        enddo
```

# The first simulation: radioactive decay

- implement algo into a small program
- show results after 3000 sec for:

$$N_0 = 100, \ \alpha = 0.01 \ s^{-1}$$
 $\Delta t = 1s$ 
 $N_0 = 5000, \ a = 0.03 \ s^{-1}$ 
 $\Delta t = 1s$ 

- MC experiment does not excatly 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  $u_i$ :

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

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

Convergence

is given with a certain probability ...

BUT is a mathematically serious and precise statement

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**BUT** is a mathematically serious and precise statement

Gambling in Monte Carlo is also serious and sophisticated Some people say

### 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

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

### **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:

$$R_n = \sum_{i=1}^n R_i$$

$$E(R_1) = \int u du = 1/2,$$

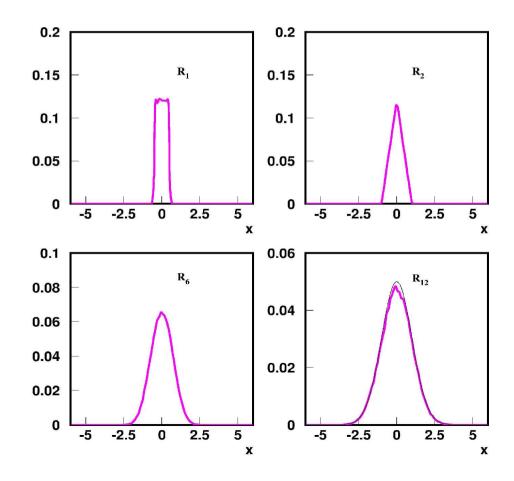
$$V(R_1) = \int (u - 1/2)^2 du = 1/12$$

$$E(R_n) = n/2$$

$$V(R_n) = n/12$$

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

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



### Resumee: Monte Carlo technique

Law of large numbers

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

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) decrease  $\sigma$ : reduce V(f) or increase N

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

## Monte Carlo: Buffons Needle - Hit & Miss

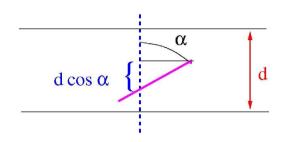
- Buffons needle (Buffon 1777)
   pattern of parallel lines with
   distance d,
   randomly throw needle with length d
   onto stripes,
   count hit, when needle crosses strip
   count miss, if not
- probability for hit is:

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

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/buff.html



```
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*ntrial/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

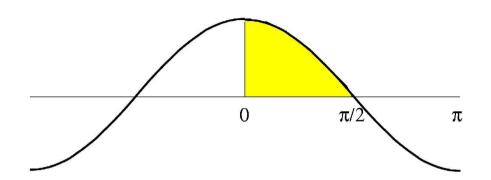
$$\int_0^{\pi/2} \cos(\alpha) d\alpha$$

apply Law of large numbers:

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

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
10000000	3.12174	3.14156

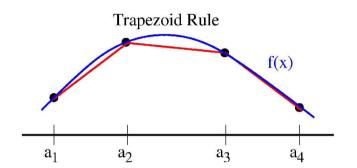
### Integration: Monte Carlo versus others

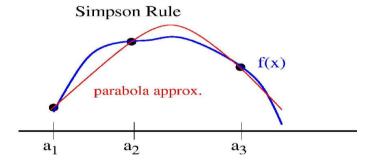
#### One dimensional quadrature

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

- 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





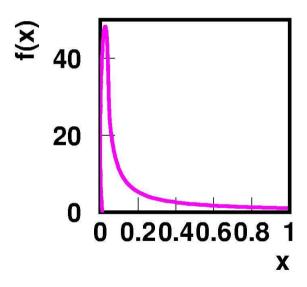
method	err(1d)	error
MC	<b>n</b> <sup>-1/2</sup>	<i>n</i> <sup>-1/2</sup>
Trapez	<b>n</b> -2	<b>n</b> -2/d
Simpson	<i>n</i> -4	<b>n</b> -4/d
Gauss	<b>n</b> -2m+1	<b>n</b> -(2m-1)/a

- integration 
   weighting events
   large fluctuations from large weights
   weights also to errors applied
   difficult to apply further hadronisation
- real events all have weight = 1  $\frac{111}{111}$
- Hit & Miss method:

MC for function f(x):
get random number:
R1 in (0,1) and R2 in (0,1)calculate x = R1reject event if:  $f_x < f_{max} R2$ 

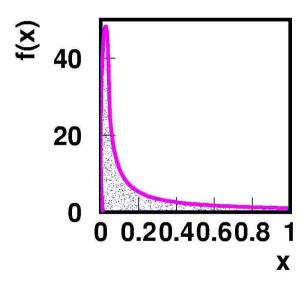
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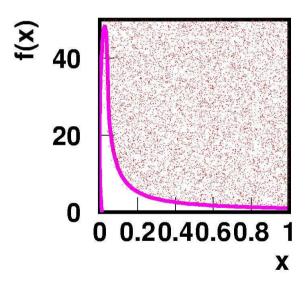
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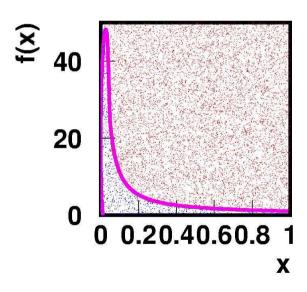
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• BUT: Hit & Miss method inefficient for peaked f(x)

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

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

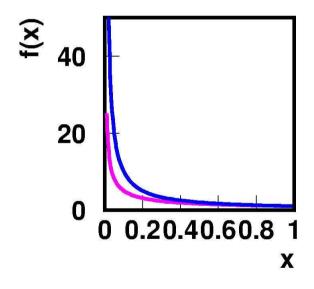
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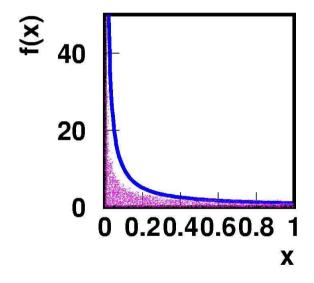
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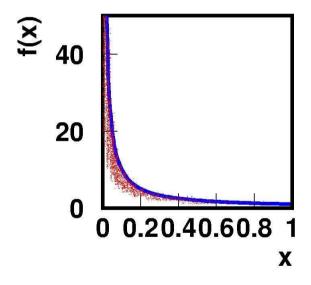
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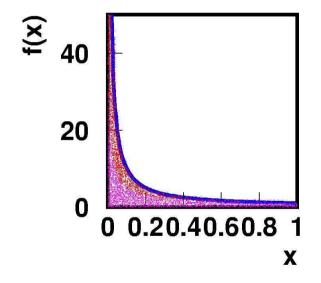
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• WOW  $\coprod$  very efficient even for peaked f(x)

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

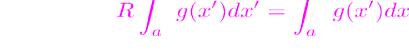
# Importance Sampling

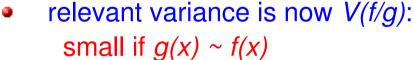
MC calculations most efficient for small weight fluctuations:

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

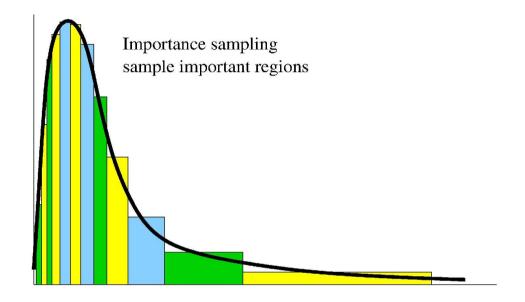
- chose point according to g(x) instead of uniformly
- f is divided by g(x) = dG(x)/dx
- generate x according to:

$$R \int_{a}^{b} g(x')dx' = \int_{a}^{x} g(x')dx'$$





- how-to get g(x)
  - (1) g(x) is probability: g(x) > 0 and  $\int dG(x) = 1$
  - (2) integral  $\int dG(x)$  is known analytically
  - (3) G(x) can be inverted (solved for x)
  - (4) 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<sup>+</sup>e<sup>-</sup>
- what about hadronsiation
- what about QCD radiation
- going even further: initial state radiation
- how-to do a DIS Monte Carlo event generator
- some examples

# Application of MC method: Compton scattering

Compton scattering (O. Klein, Y. Nishima, Z. Physik, 52, 853 (1929))
 energy of the final photon k':

$$k' = \frac{k}{1 + (k/m)(1 - \cos\theta)} \qquad \sum_{k}^{k} \sum_{k}^{k'} \sum_{k}^{m} \frac{k'}{2} \sum_{k}^{m} \frac{k'}{$$

Differential cross section

$$rac{d\sigma}{d\Omega} = rac{lpha_{em}^2}{2m^2} \left(rac{k'}{k}
ight)^2 \left(rac{k'}{k} + rac{k}{k'} - \sin^2 heta
ight)$$

angular distribution of the photon is:

$$\sigma(\theta,\phi)d\theta d\phi = \frac{\alpha_{em}^2}{2m^2} \left( \left( \frac{k'}{k} \right)^3 + \left( \frac{k}{k'} \right) - \left( \frac{k'}{k} \right)^2 \sin^2 \theta \right) \sin \theta d\theta d\phi$$

• generate azimuthal  $\phi$  independently:  $\phi = 2 \pi R_1$ 

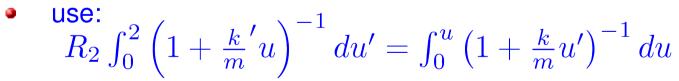
#### Application of MC method: Compton scattering

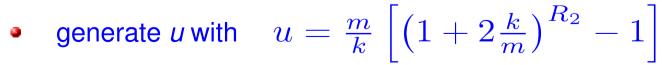
• to generate  $\theta$ , use approximation for  $k \gg m$ , x-section peaked at small angles (using  $u=(1-\cos\theta)$ ):

$$\sigma^{a}d\theta d\phi = \frac{\alpha_{em}^{2}}{2m^{2}} \left(\frac{k'}{k}\right) \sin\theta d\theta d\phi$$

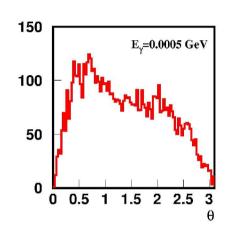
using 
$$k' = \frac{k}{1 + (k/m)(1 - \cos \theta)}$$

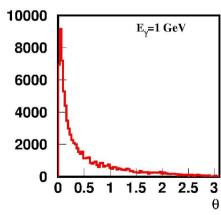
$$\sigma^a d heta d\phi = rac{lpha_{em}^2}{2m^2} \left(1 + rac{k}{m}u
ight)^{-1} du d\phi$$











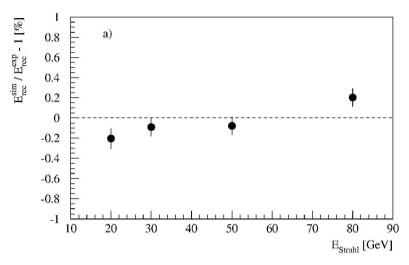
#### Application of MC method: photon transport in matter

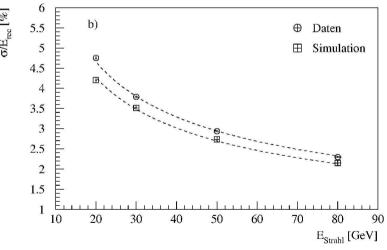
Program for Compton scattering and similar programs for photo-effect and paircreation build program that simulates interactions of photons with matter

- Algorithm
  - break path into small pieces
  - in each step, decide whether interaction (and which) takes place, given the total cross section for each possible interaction
  - from mean free path length, decide where interaction takes place
  - simulate interaction: give photon new energy and angle, or produce  $e^+e^-$  pair, etc ...
  - continue path with new parameters
- such program exist
  - EGS (SLAC)
  - GEANT (CERN)
- Detector simulation with programs for particle transport in matter
  - to study detector design
  - to obtain a detailed simulation of the detector response
  - to estimate efficiencies, bias, etc...

#### Application of Simulation: Calibration of H1 Calorimeter

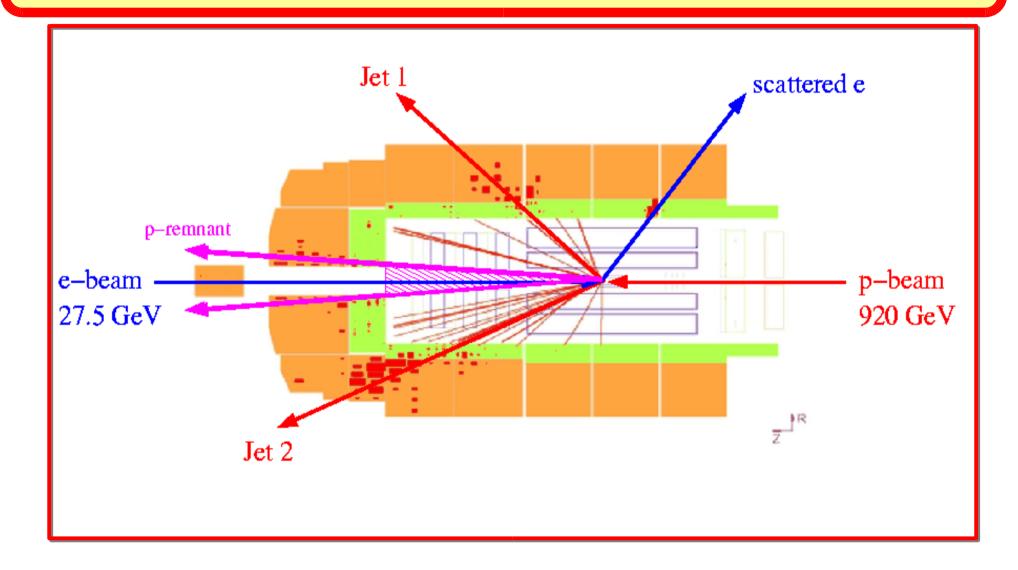
- simulated energy response in calorimeter using GEANT package including full detector geometry and material information
- test beam measurement of energy response
- test of understanding detector performance
- nice agreement within ~ 3%
- difference due to dead material in front of detector





J. Spiekermann, diploma 1994

# MC event: hadron and detector level



 $\sqrt{s} \sim 318 \text{ GeV} \rightarrow x \sim 7. \ 10^{-5} \text{ at } Q^2 = 4 \text{ GeV}^2$ 

## 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 to correct from detector to hadron level

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

visible x-section on hadron level

All measurements rely on proper MC's !!!



## MC generators - different applications ...

- calculate x-section of various processes roughlicated 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
```

H. Jung, Summerstudent Lecture 2005

integration of multidimensional phase space

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

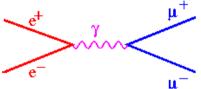
- $\frac{d\sigma}{d\cos\theta d\phi} = \frac{\alpha_{em}^2}{4s} \left(1 + \cos^2\theta\right)$
- goal: generate 4-momenta of  $\mu$ 's, need cm energy s,  $cos \theta$ ,  $\phi$

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

- for every R1, R2 use weight with
- repeat many times

 $\frac{d\,\sigma}{d\cos\theta\,d\,\phi}$ 

process: e<sup>+</sup>e<sup>-</sup> → μ<sup>+</sup> μ<sup>-</sup>



 $d\sigma$ 

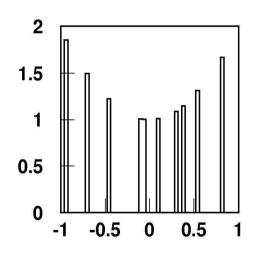
 $d\cos\theta d\phi$ 

- $\frac{d\sigma}{d\cos\theta d\phi} = \frac{\alpha_{em}^2}{4s} \left(1 + \cos^2\theta\right)$
- goal: generate 4-momenta of  $\mu$ 's, need cm energy s,  $cos \theta$ ,  $\phi$

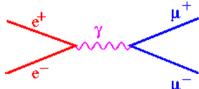
random number R1(0,1)  $\phi$  = 2  $\pi$  R1 random number R2(0,1) cos  $\theta$  = -1 + 2 R2

- for every R1, R2 use weight with
- repeat many times

#### after 10 events



process: e<sup>+</sup>e<sup>-</sup> → μ<sup>+</sup> μ<sup>-</sup>

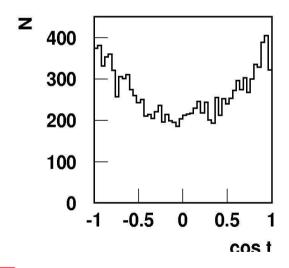


- $\frac{d\sigma}{d\cos\theta d\phi} = \frac{lpha_{em}^2}{4s} \left(1 + \cos^2 heta
  ight)$
- goal: generate 4-momenta of  $\mu$ 's, need *cm* energy *s*,  $\cos \theta$ ,  $\phi$

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

- for every R1, R2 use weight with
- repeat many times

#### after 10000 events

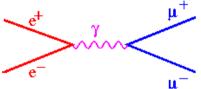


H. Jung, Summerstudent Lecture 2005

 $d\sigma$ 

 $d\cos\theta d\phi$ 

process: e<sup>+</sup>e<sup>-</sup> → μ<sup>+</sup> μ<sup>-</sup>



- $\frac{d\sigma}{d\cos\theta d\phi} = \frac{lpha_{em}^2}{4s} \left(1 + \cos^2 heta
  ight)$
- goal: generate 4-momenta of  $\mu$ 's, need *cm* energy *s*,  $\cos \theta$ ,  $\phi$

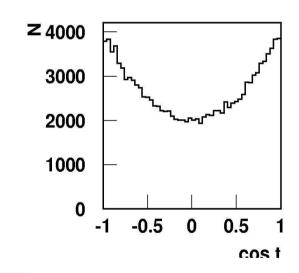
random number R1(0,1)  $\phi$  = 2  $\pi$  R1 random number R2(0,1) cos  $\theta$  = -1 + 2 R2

for every R1, R2 use weight with

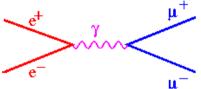
repeat many times

 $\frac{d\,\sigma}{d\cos\theta\,d\,\phi}$ 

#### after 100000 events



process: e<sup>+</sup>e<sup>-</sup> → μ<sup>+</sup> μ<sup>-</sup>



- $\frac{d\sigma}{d\cos\theta d\phi} = \frac{\alpha_{em}^2}{4s} \left(1 + \cos^2\theta\right)$
- 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 + 2 R2

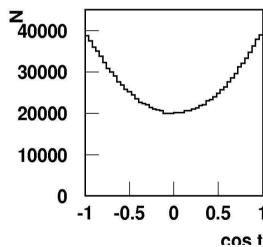
for every R1, R2 use weight with

repeat many times

dσ

 $d\cos\theta d\phi$ 

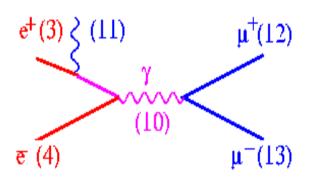
#### after 10<sup>6</sup> events



## Example event: e⁺e⁻ → µ⁺ µ⁻

#### example from PYTHIA: Event listing

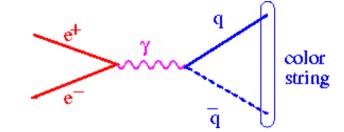
I particle/	jet KS	KF c	rig	p_x	р_у	p_z	E	m
1 !e+! 2 !e-!	21 21	-11 11	0	0.000	0.000	30.000	30.000	0.001
3 !e+! 4 !e-! 5 !e+! 6 !e-! 7 !Z0! 8 !mu-! 9 !mu+!	21 21 21 21 21 21 21 21	-11 11 -11 11 23 13 -13	1 2 3 4 0 7	0.000 0.000 0.143 0.000 0.143 -9.510 9.653	0.000 0.000 0.040 0.000 0.040 1.741 -1.700	30.000 -30.000 26.460 -29.998 -3.539 24.722 -28.261	30.000 30.000 26.460 29.998 56.458 26.546 29.913	0.000 0.000 0.000 0.000 56.347 0.106 0.106
10 (ZO) 11 gamma 12 mu- 13 mu+	======== 11 1 1 1 ====================	23 22 13 -13 -20 0.00	====== 7 3 8 9 ======	0.143 -0.143 -9.510 9.653 	0.040 -0.040 1.741 -1.700 ======== 0.000	-3.539 3.539 24.722 -28.261 ======== 0.000	56.458 3.542 26.546 29.913 ======== 60.000	56.347 0.000 0.106 0.106 ======= 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 $e^+e^- o q\bar{q}$

- process  $e^+e^- \rightarrow q\bar{q}$
- $\frac{d\sigma}{d\cos\theta d\phi} = \frac{\alpha_{em}^2}{4s} \left(1 + \cos^2\theta\right) \qquad e^{-\frac{\theta}{2}}$



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

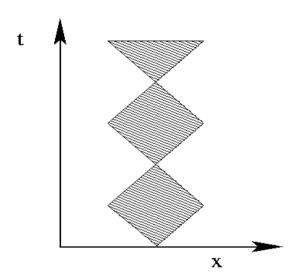
linear confinement potential:  $V(r) \sim -1/r + \kappa r$ with  $\kappa \sim 1 \text{ GeV/fm}$ 

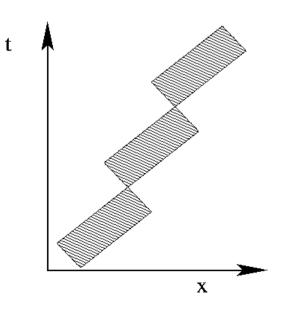
qq connected via color flux tube of transverse size of hadrons (~1 fm) color tube: uniform along its length → linearly rising potential

→ 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, with a string tension of:
   κ~1GeV/fm~0.2 GeV²
- as q and q 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





# Lund string fragmentation (cont'd)

- color force materialise a massless qq pair on a point on the string
- string separates into two independent (color neutral) strings analogy with electric filed coupled to particles suggest:

$$\frac{dP}{dxdt} = C \exp\left(\frac{-\pi m^2}{\kappa}\right)$$

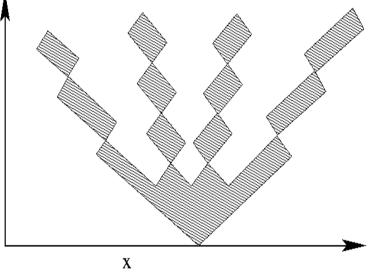
... tunneling probability through potential barrier

production of different flavour in hadronization

$$P \propto \exp\left(\frac{-\pi m^2}{\kappa}\right)$$

with 
$$m_u = m_d = 0$$
,  $m_s = 0.25 \,\text{GeV}$ ,  $m_c = 1.2 \,\text{GeV}$   
 $u:d:s:c = 1:1:0.37:10^{-10}$ 

typical example of Monte Carlo approach



# 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)

$$P \sim \exp\left(-\frac{\pi m_t^2}{\kappa}\right) = \exp\left(-\frac{\pi m^2}{\kappa}\right) \exp\left(-\frac{\pi p_t^2}{\kappa}\right)$$

- suppression of heavy quark production
   u:d:s:c ~ 1:1:1:0.37:10<sup>-10</sup>
   actually leave it as a free parameter
- longitudinal fragmentation symmetric fragmentation function (from either q or q)  $f(z) \sim z^{-1}(1-z)^a \exp(-b m_t^2/z)$ 
  - harder spectrum for heavy quarks
- start from q or q
- repeat until cutoff is reached
- heavy use of random numbers and importance sampling method

 $\frac{rp_t^2}{\kappa}$  (transverse frag.

longitudinal frag.

## Particles and Decays

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

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

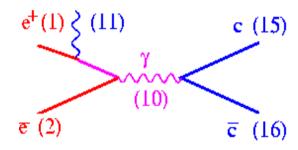
- lifetimes
  - related to widths ... but for practical purpose separated
  - $\rightarrow$   $P(\tau)d\tau \sim exp(-\tau/\tau_0)d\tau$
  - calculate new vertex position  $v' = v + \tau p/m$
- decays
  - taken from PDG, where known

  - assume momentum distribution given by phase space only exceptions, like  $\omega, \phi \to \pi^+\pi^-\pi^0$ , or  $D \to K\pi, D^* \to K\pi\pi$ and some semileptonic decays use matrix elements

# Example event e⁺e⁻ → qq

example from PYTHIA Monte Carlo generator including hadronization

I particle/je	et KS	KF	orig	p_x	р_у	p_z	E	m
1 !e+! 2 !e-!	21 21	-11 11	0 0	0.000	0.000	30.000 -30.000	30.000	0.001 0.001
5 !e+! 6 !e-!	21 21	-11 11	3 4	0.018 0.000	0.040 0.000	0.702	0.703 29.998	0.000
10 (ZO) 11 gamma 15 (c) A 16 (cbar) V		23 22 4 -4	7 1 10 10	0.018 -0.018 -1.950 1.967	0.040 -0.040 -3.529 3.569	-29.297 29.298 -19.752 -9.545	30.701 29.298 20.215 10.486	9.180 0.000 1.500 1.500
17 (string) 18 (D0) 19 (omega) 20 pi+ 21 (rho-) 22 (omega) 23 pi+ 24 (D*-) 25 e+ 26 nu_e	11 11 11 11 11 11 11 11 11	92 421 223 211 -213 223 211 -413 -11	15 17 17 17 17 17 17 17 17	0.018 -0.455 -0.300 -0.168 -0.114 -0.173 0.226 1.001 -0.191 -0.154	0.040 -1.495 -0.076 -0.172 -0.513 0.118 0.925 1.253 0.241 -0.789	-29.297 -9.002 -3.228 -0.861 -4.992 -2.022 -2.593 -6.599 -1.261 -4.174	30.701 9.325 3.338 0.904 5.106 2.180 2.766 7.082 1.297 4.250	9.180 1.865 0.793 0.140 0.932 0.789 0.140 2.010 0.001 0.000
 53 pi-	1 ====== sum:	-211 -===== 0.00	47 =====	0.318 ======= 0.000	-0.061 ====== 0.000	-1.293 ======== 0.000	1.340 ====================================	0.140 ====== 60.000

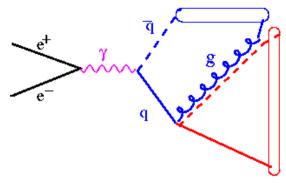


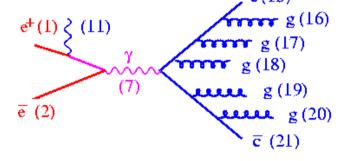
- apply fragmentation directly to parton all covered by hadronization .... soft
- where is QCD ???

# Doing things better: e⁺e⁻ → qqg

- process e<sup>+</sup>e<sup>-</sup> → qqg
- full matrix element calculation
- watch out color flow !!!
- gluons act as kicks on strings

I	particle/je	t KS	KF	orig	p_x	р_у	p_z	E	m
	!e+! !e-!	21 21	-11 11	0	0.000	0.000	30.000 -30.000	30.000	0.001
=====		=====	======	=====	=======	=======	=======	=======	======
5	!e+!	21	-11	1	0.000	0.000	29.699	29.699	0.000
6	!e-!	21	11	2	-1.319	-1.236	-26.950	27.011	0.000
7	!Z0!	21	23	0	-1.319	-1.236	2.748	56.710	56.614
8	!c!	21	4	7	-15.986	16.072	18.293	29.167	1.500
9	!cbar!	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	8	-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	0.179	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	-0.364	0.835	0.000
21	(g) I	12	21	9	8.331	-6.743	-6.396	12.482	0.000
2.2	(cbar) V	11	-4	9	5.754	-8.971	-8.335	13.613	1.500

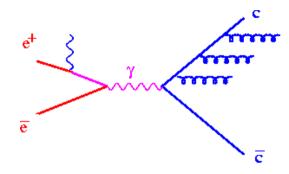




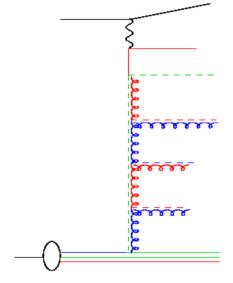
- more large p<sub>t</sub> emissions
- not all covered by fixed order calculations
- doing much better needed
- parton shower approach

#### Approximations to higher orders: parton showers

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



parton density functions



- since alphas 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  $q \frac{\partial}{\partial q} f(x,q) = \int \frac{dz}{z} \, \frac{lpha_s}{2\pi} P_+(z) \, f\left(\frac{x}{z},q\right)$ 

modified differential form using "Sudakov form factor"

$$\Delta_{s}(q_{0},q) = \exp\left(-\bar{\alpha}_{s} \int \frac{dz}{z} \int_{q_{0}}^{q} \frac{dq'}{q'} \tilde{P}(z)\right)$$

$$q \frac{\partial}{\partial q} \frac{f(x,q)}{\Delta_{s}(q,q_{0})} = \int \frac{dz}{z} \frac{\alpha_{s}}{2\pi} \frac{\tilde{P}(z)}{\Delta_{s}(q,q_{0})} f\left(\frac{x}{z},q\right)$$

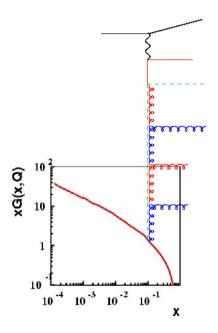
integral form

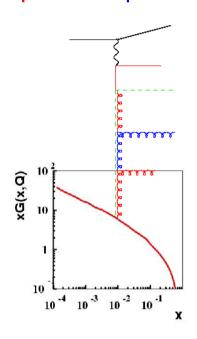
$$f(x,q) = f_0(x,q)\Delta_s(q,q_0) + \int \frac{dz}{z} \int \frac{dq'}{q'} \cdot \Delta_s(q',q_0)\tilde{P}(z)f\left(\frac{x}{z},q\right)$$

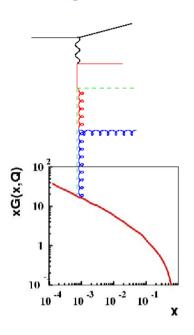
no-branching probability form q<sub>0</sub> to q

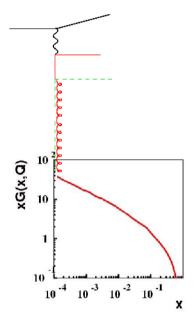
## DGLAP evolution equation

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









$$f(x,Q) = f_0(x,q_0)\Delta_s(Q,q_0) + \sum_{k=1}^{\infty} f_k(x_k,q_k)$$

## Parton Showers for the final state

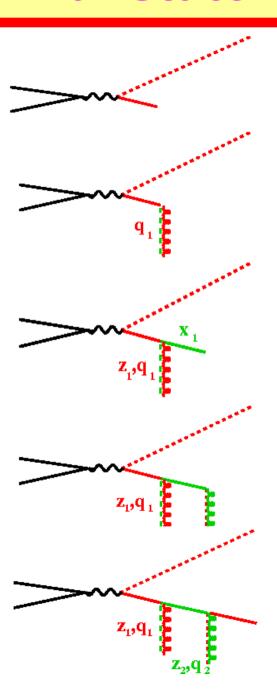
#### timelike parton shower evolution

- starting with hard scattering
- select q<sub>1</sub> from Sudakov form factor

select z<sub>1</sub> from splitting function

select q<sub>2</sub> from Sudakov form factor

- select z<sub>2</sub> from splitting function
- stop evolution if  $q_2 < q_0$



## Parton Shower

- Evolution equation with Sudakov form factor recovers exactly evolution equation (with prescription)
- Sudakov form factor particularly suited form Monte Carlo approach
- Sudakov form factor
  - $\rightarrow$  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 ~ p,
- need to specify cutoff scale  $Q_0 \sim 1 \text{ GeV}$

## The DIS process ep → epX

oross section  $\frac{d\sigma(ep\to e'X)}{dy\,dQ^2}=\frac{4\pi\alpha^2}{yQ^4}\left(\left(1-y+\frac{y^2}{2}\right)F_2^p(x,Q^2)-\frac{y^2}{2}F_L^p(x,Q^2)\right)$  with  $F_2^p(x,Q^2)=\sum_f e_f^2\left(xq_f(x,Q^2)+x\bar{q}_f(x,Q^2)\right)$ 

• generate y with g(y)=1/y, and  $Q^2$  with  $g(Q^2)=1/Q^2$ :

$$y = y_{min} \left(\frac{y_{max}}{y_{min}}\right)^{R_1}$$

$$Q^2 = Q_{min}^2 \left(\frac{Q_{max}^2}{Q_{min}^2}\right)^{R_2}$$

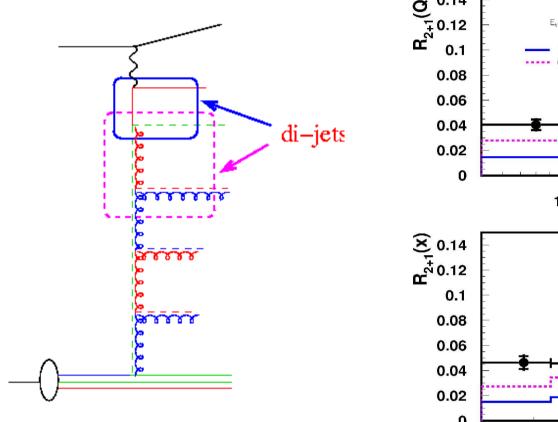
calculate x-section with:

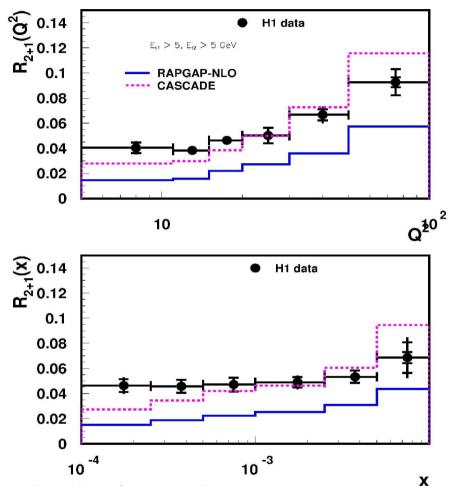
$$\sigma(ep \to e'X) = \frac{1}{N} \sum_{i=1}^{N} \frac{\frac{a\sigma}{dy_i dQ_i^2}}{g(y_i)g(Q_i^2)} \int g(y)dy \int g(Q^2)dQ^2$$

$$\sigma(ep \to e'X) = \frac{1}{N} \sum_{i=1}^{N} \frac{y_i Q_i^2}{dy_i dQ_i^2} \log\left(\frac{y_{max}}{y_{min}}\right) \log\left(\frac{Q_{max}^2}{Q_{min}^2}\right)$$

calculate 4-momenta of scattered electron and virtual photon

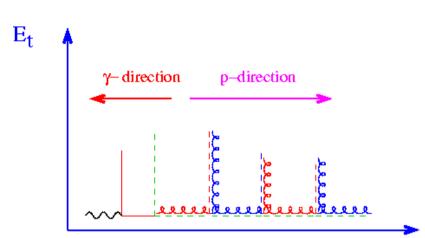
## Hadronic final state: Di-jet rates



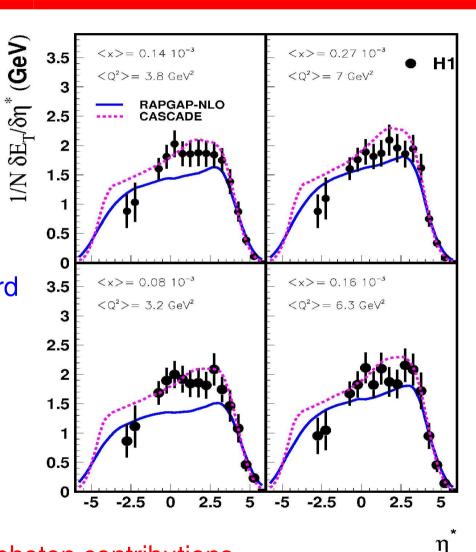


- (2+remnant) jets in DIS for  $Q^2 > 5 \text{ GeV}^2$ ,  $p_t^{\text{jets}} > 5 \text{ GeV}$
- $\mathcal{O}(\alpha_s)$  processes not enough
  - $\rightarrow$  need  $\mathcal{O}(\alpha_s^2)$  or resolved virtual photon contributions
  - → or something new ???

## Hadronic final state: Energy flow



- Et flow in DIS at small x and forward angle (p-direction):
- $\rightarrow \mathcal{O}(\alpha_s)$  processes not enough



- need  $\mathcal{O}(\alpha_s^2)$  or resolved virtual photon contributions
- or something new ???

### 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, hadronziation not enough
- MC approach extended from simple e+e- processes to ep processes pp processes and heavy lon 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 program

- HERA Monte Carlo workshop: 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.

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.

## List of available MC program

#### 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.

#### 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.