Introduction to Monte Carlo generators
(Fully exclusive modeling of high-energy collisions)

Andrzej Siodmok

CTEQ School - University of Pittsburgh, USA 18 - 28 July 2017

2008 CTEQ - MCnet Summer School on QCD Phenomenology and Monte Carlo Event Generators

Lectures:
- Jet Physics
- Heavy Quarks
- Standard Model
- Event Generators in Use
- Introduction to QCD
- Event Generators in LHC
- Deep Inelastic Scattering
- Heavy Flavor Production
- Parton Distribution Functions
- Vector Boson Production
- Monte Carlo in Medical Research
- Matrix Element Matching Methods

A combination of broad lectures on QCD theory, phenomenology, and analyses and a practical approach to event generation. Physics and techniques, with hands-on sessions included in using them in real analyses.

Sponsors are available for participants from less favoured regions and new member states of the EU and others in financial need. Applications are particularly encouraged from women and other under-represented sections of the community.

Local Organizing Committee: Zsolt Toth

Website:
www.cteq-mcnet.org

2010 CTEQ - MCnet Summer School on QCD Phenomenology and Monte Carlo Event Generators

Lauterbad (Black Forest) Germany
26 July - 4 August 2010

Lectures:
- 8-Physics
- Jet Physics
- Deep Inelastic Scattering
- Heavy Flavor Production
- Top Quark Physics
- Standard Model and Higgs
- Parton Distribution Functions
- Vector Boson Production
- Direct and Indirect Methods
- Introduction to Monte Carlo Event Generators
- Introduction to the PHOTOS and SHERPA QCD

First LHC Results:
- High pt
- Minimum Bias
- Small X and PDFs
- Low pt and Particle ID

Event Generation and First Hands-on Practice

Bursaries are available for participants from less favoured regions and new member states of the EU and others in financial need. Applications are particularly encouraged from women and other under-represented sections of the community.

Sponsors:
- Fermilab
- US National Science Foundation
- Kavli Institute of Technology
- Deutsches Elektronen-Synchrotron
- Helmholtz Alliance "Physics at the Terascale"
- European Organization for Nuclear Research
- EU Marie Curie Actions: Human Resources and Mobility

Website:
www.cteq-mcnet.org
There is a huge gap between a one-line formula of a fundamental theory, like the Lagrangian of the SM, and the experimental reality that it implies.
Motivation

General Purpose Monte Carlo (GPMC) event generators are designed to bridge that gap.

One can think of a GPMC as a “Virtual Collider” ⇒ Direct comparison with the data.

Almost all HEP measurements and discoveries in the modern era have relied on GPMC generators, most notably the discovery of the Higgs boson.

DATA MAKES YOU SMARTER

It doesn’t matter how beautiful your theory is, it doesn’t matter how smart you are. If it doesn’t agree with experiment, it’s wrong.

Richard P. Feynman

Detector simulation
Pions, Kaons, ...
Reconstruction
B-tagging efficiency
Boosted decision tree
Neural network

...
General Purpose Monte Carlo (GPMC) event generators are designed to bridge that gap.

Theory
- Lagrangian
- Gauge invariance
- QCD
- Partons
- NLO
- Resummation
  ...

MC event generators

Experiment
- Detector simulation
- Pions, Kaons, ...
- Reconstruction
- B-tagging efficiency
- Boosted decision tree
- Neural network
  ...

Motivation
General Purpose Monte Carlo (GPMC) event generators are designed to bridge that gap.

One can think of a GPMC as a “Virtual Collider” \(\Rightarrow\) Direct comparison with the data.

Almost all HEP measurements and discoveries in the modern era have relied on GPMC generators, most notably the discovery of the Higgs boson.
Real vs Virtual

real life

Machine
LHC, Tevatron ...

Detector, Data Acquisition
CMS, ATLAS, CDF ...

virtual reality

Event Generator
Herwig, Pythia, Sherpa ...

Detector Simulation
Geant 4 ...

Event Reconstruction
ORCA ...

Analysis
ROOT ...

quick and dirty
Monte Carlo simulations are used by all experimental collaborations both to compare their data and theoretical predictions, and in data analysis.

Unfortunately they are often treated as black boxes ...

J. D. Bjorken

“But it often happens that the physics simulations provided by the MC generators carry the authority of data itself. They look like data and feel like data, and if one is not careful they are accepted as if they were data.”

It’s important to understand the assumptions and approximations involved in these simulations.

It is important to understand what is inside the programs to be able to answer the following type of questions.

- Is the effect I’m seeing due to different models (important to use more than one generator!), or approximations, or is it a bug?
- Am I measuring a fundamental quantity or merely a parameter in the simulation code?
What do MC event generators do?

- An “event” is a list of particles (pions, protons, ...) with their momenta.
- The MCs generate events.
- The probability to generate an event is proportional to the (approximate!) cross section for such an event.
- Calculate Everything \( \sim \) solve QCD (1M $ prize) \rightarrow \) requires compromise!
- Improve lowest-order perturbation theory, by including the “most significant” corrections \( \rightarrow \) complete events (can evaluate any observable you want)

The Workhorses: What are the Differences?

All offer convenient frameworks for LHC physics studies, but with slightly different emphasis:

**PYTHIA**: Successor to JETSET (begun in 1978). Originated in hadronization studies: Lund String.


**SHERPA**: Begun in 2000. Originated in “matching” of matrix elements to showers: CKKW.
What do parton shower event generators do?

2012 J.J. Sakurai Prize for Theoretical Particle Physics Recipient

The 2012 Sakurai Prize is awarded to:

- Guido Altarelli (Università di Roma Tre)
- Torbjorn Sjostrand (Lund University)
- Bryan Webber (University of Cambridge)

for key ideas leading to the detailed confirmation of the Standard Model of particle physics, enabling high energy experiments to extract precise information about quantum chromodynamics, electroweak interactions, and possible new physics.
Parton Distribution Function - see P. Nadolsky lectures
Hard process (exact fixed-order perturbation theory - R. Boughezal lecture)
Parton Shower (Approximate all-order perturbation theory)
Parton Shower (Approximate all-order perturbation theory)
Hadronization (non-perturbative semi-empirical models)
Hadron decay - PDG book
Multiple Interactions and beam remnants
Literature

- R. K. Ellis, W. J. Stirling, B. R. Webber
  QCD and Collider Physics
  Cambridge University Press, 2003

- T. Sjöstrand, S. Mrenna, P. Z. Skands
  PYTHIA 6.4 Physics and Manual
  JHEP 05 (2006) 026

- A. Buckley et al.
  General-Purpose Event Generators for LHC Physics
  Phys. Rept. 504 (2011) 145

- R. D. Field
  Applications of Perturbative QCD
  Addison-Wesley, 1995
Plan

▶ 1st lecture
  ▶ Monte Carlo methods why and how?
  ▶ Parton Shower

▶ 1st tutorial
  ▶ Build your own Parton Shower (in Python)!

▶ 2nd lecture
  ▶ Hadronization
  ▶ Multiple Parton Interaction
  ▶ Tuning

▶ 2nd tutorial
  ▶ Shower uncertainties (in Python)
    or
  ▶ MC@NLO/POWHEG (see Marek’s lecture) matching in Python

▶ 3rd tutorial
  ▶ Real life example - work with Herwig, Sherpa and Pythia!
We want to compute expectation values of observables
\[ \langle O \rangle = \sum_n \int d\phi_n P(\phi_n) O(\phi_n), \]
where \( \phi_n \) - Point in n-particle phase-space, \( P(\phi_n) \) Probability to produce \( \phi_n \), Value of observable at \( O(\phi_n) \).

large \( n \) \( \mathcal{O}(100 \div 1000) \) \( \Rightarrow \) Monte Carlo is the only choice.
Why they are called Monte Carlo Event Generators?

\[ \langle O \rangle = \sum_n \int d\phi_n P(\phi_n) O(\phi_n) \]

Problems:

- Integrate a multi dimensional function
- Pick a point at random according to a probability distribution
- Problems with “memory”, eg.: Radioactive decay

Integrate a function

<table>
<thead>
<tr>
<th>Numerical Integration: Relative Uncertainty (after ( n ) function evaluations)</th>
<th>( n_{\text{eval}} / \text{bin} )</th>
<th>One Dimension Conv. Rate</th>
<th>D Dimensions Conv. Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trapezoidal Rule (2-point)</td>
<td>( 2^D )</td>
<td>( 1/n^2 )</td>
<td>( 1/n^{2/D} )</td>
</tr>
<tr>
<td>Simpson’s Rule (3-point)</td>
<td>( 3^D )</td>
<td>( 1/n^4 )</td>
<td>( 1/n^{4/D} )</td>
</tr>
<tr>
<td>Monte Carlo</td>
<td>1</td>
<td>( 1/n^{1/2} )</td>
<td>( 1/n^{1/2} )</td>
</tr>
</tbody>
</table>

+ optimisations (stratification, adaptation), iterative solutions (Markov-Chain Monte Carlo)
Monte Carlo methods are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results.

Examples:

- **Buffon’s needle, 18th century by Georges-Louis Leclerc**,  
  Calculate $\pi$ by dropping a needle onto the floor.  
  $\leftarrow 34/11 \sim 3.1$ based on 17 throws

- **Lord Kelvin (1901)** – use random sampling (drawing numbered pieces of paper from a bowl) to aid in evaluating some integrals in the kinetic theory of gases.
MC examples

- Enrico Fermi (1930s) – numerical sampling experiments on neutron diffusion and transport in nuclear reactors (device FERMIAC – a mechanical sampling device).

- Project Manhattan (nuclear weapons projects) - S. Ulam, J. von Neumann. Name Monte Carlo refers to the Monte Carlo Casino in Monaco where Ulam’s uncle would borrow money from relatives to gamble.

- In Particle Physics we have to solve multidimensional integrals (many particles) MC methods very efficient! So we play roulette to understand low of the nature :)
The **distribution of a random variable** gives the probability of a given value (or infinitesimal range of values).

For continuous variables we define

\[ \rho(u) du = \mathcal{P}[u < u' < u + du], \]

\( \rho(u) \) – **the probability density function (pdf)** of \( u \) (gives the probability of finding the random variable \( u' \) within \( du \) of a given value \( u \)).

The **cumulative (integrated) distribution function (cdf)**:

\[ R(u) = \int_{-\infty}^{u} \rho(x) dx, \quad \rho(u) = \frac{dR(u)}{du}. \]

Note: \( R(u) \) – monotonically non-decreasing function and \( 0 \leq R(u) \leq 1 \).

**Expectation value of a function** \( f(u') \):

\[ E(f) = \int f(u) dR(u) = \int f(u) \rho(u) du. \]

If \( u' \in \mathcal{U}(0, 1) \), i.e. uniformly distributed between 0 and 1, then

\[ E(f) = \int_{0}^{1} f(u) du \] **Variance of a function** \( f(u') \):

\[ V(f) = E[f - E(f)]^2 = \int [f - E(f)]^2 dR = E(f^2) - E^2(f). \]

⇒ **Standard deviation**: \( \sigma(f) = \sqrt{V(f)} \).
1. **The Law of Large Numbers (LLN)** Let’s choose \( n \) numbers \( u_i \) randomly with a probability density uniform on the interval \((a, b)\), and for each \( u_i \) evaluate the function \( f(u_i) \). Then, as \( n \) becomes large:

\[
\frac{1}{n} \sum_{i=1}^{n} f(u_i) \xrightarrow{n \to \infty} E(f) = \frac{1}{b - a} \int_a^b f(u)du.
\]

2. **The Central Limit Theorem** (MC precision is stochastic: 1/\( \sqrt{n} \))

The sum of a large number of independent random variables is always normally distributed (i.e. a Gaussian distribution), no matter how the individual random variables are distributed, provided they have finite expectations and variances and provided \( n \) is ‘large enough’.

\[
\Downarrow
\]

The MC estimate is Gauss distributed around the true value with \( \sqrt{V(f)}/\sqrt{n} \) precision.
In practice the CLT convergence is pretty fast. The illustration of CLT for \( x_i \in \mathcal{U}(0, 1), i = 1, \ldots, 12: \)
Non-uniform random number generation

Random numbers of distributions other than uniform are usually obtained from uniformly distributed random numbers by applying some transformation methods.

Gaussian random number generator based on the CLT:
Let $x_i \in \mathcal{U}(0, 1)$, $i = 1, \ldots, n$, take $R_n = \sum_{i=1}^{n} x_i$, then:

\[
\begin{align*}
E(x_i) &= \frac{1}{2} \\
V(x_i) &= \frac{1}{12}
\end{align*}
\]

\[
E(R_n) = \frac{n}{2}, \quad V(R_n) = \frac{n}{12}
\]

→ From the above we have:

\[
\frac{R_n - n/2}{\sqrt{n/12}} \xrightarrow[n \to \infty]{} N(0, 1),
\]

i.e. we get the standardized Gaussian random number generator.

A convenient choice for practical purposes is:

\[n = 12 \quad \rightarrow \quad R_{12} - 6.\]

Warning: The tails of the Gaussian distribution are not well reproduced by this kind of a generator!
Inverse transform method:
Let \( U \) – uniformly distributed random number over \((0, 1)\), i.e. \( U \in \mathcal{U}(0, 1) \), and \( F \) – some continuous and increasing cumulative distribution function. Then the random variable

\[
X = F^{-1}(U)
\]

is distributed according to the cumulative distribution function \( F(x) \).

Proof: \( \mathcal{P}[X \leq x] = \mathcal{P}[F^{-1}(U) \leq x] = \mathcal{P}[U \leq F(x)] = F(x) \).

Example:

Exponential distribution \( E(0, 1) \rightarrow \text{pdf: } \rho(x) = e^{-x}, \ x > 0 \)

\[
\Rightarrow \text{cdf: } F(x) = \int_0^x e^{-x'} \, dx' = 1 - e^{-x}
\]

Let \( r \in \mathcal{U}(0, 1): \quad r = F(x) = 1 - e^{-x} \quad \Rightarrow \quad x = -\ln(1 - r) \), If \( r \in \mathcal{U}(0, 1) \), then \( 1 - r \in \mathcal{U}(0, 1) \) \( \Rightarrow \quad x = -\ln r \).

The method applies if both the integral of the density and its inverse are known (i.e. practically never)
Non-uniform random number generation

Rejection (hit-or-miss) method (von Neumann, 1951):
(Solution, if $F^{-1}$ is unknown.)

- Builds on “over-estimator” $g(x)$ ($G$ and $G^{-1}$ known):
  \[ g(x) > f(x) \forall x \in [x_{\text{min}}, x_{\text{max}}] \]

- Select an $x$ according to $g$ (using inverse transform method)
- Accept with probability $f(x)/g(x)$ (with another random number)

Hit and miss
$g(x) = \text{Max}_{[x_{\text{min}}, x_{\text{max}}]} f(x)$

Importance sampling
(Improved hit-and-miss)
Let:

\[ f(x) = \sum_{i=1}^{\infty} p_i g_i(x), \]

where: \( p_i \) – density of some discrete distribution, i.e. \( p_i \geq 0, \sum_{i=1}^{\infty} p_i = 1 \);

\( g_i(x) \) – some continuous pdfs.

**Generation scheme:**
A. Generate a number \( i \) according to the density \( p_i \), e.g. using the inverse transform.
B. For a given value \( i \), generate \( X \) according to the pdf \( g_i(x) \).

**Polynomial probability density functions**

\[ f(x) = \sum_{i=1}^{n} c_i x^i, \quad 0 \leq x \leq 1, \ c_i \geq 0; \quad \sum_{i=1}^{n} \frac{c_i}{i+1} = 1. \]

- A. Generate the index \( i \in \{1, 2, \ldots, n\} \) according to the pdf \( p_i = \frac{c_i}{i+1} \).

- B. For a given value \( i \) generate \( X \) according to the pdf \((i + 1)x^i\), e.g. using the inverse transform method: \( X = U^{1/(i+1)} \), where \( U \in U(0, 1) \).
Branching algorithms

The simple branching method:

\[ f(x) = \sum_{i=1}^{K} p_i g_i(x) \]

Branching and rejection:

\[ f(x) = \sum_{i=1}^{K} p_i f_i(x) \]
Radioactive decays

\[ N(t) = \text{number of remaining nuclei at time } t, \text{ normalized to } N(0) = N_0 = 1, \text{ so } N(t) = \text{probability that (single) nucleus has not decayed by time } t \]

\[ P(t) = \frac{dN(t)}{dt} = \text{probability for it to decay at time } t. \]

- No memory (wrong):
  \[ P(t) = c \Rightarrow N(t) = 1 - ct \]
  a nucleus can only decay once!

- Correct (with memory):
  \[ P(t) = cN(t) \Rightarrow N(t) = e^{-ct} \]
For radioactive decays $P(t) = cN(t)$, with $c$ constant, but now generalize to time-dependence:

$$P(t) = -\frac{dN(t)}{dt} = f(t)N(t) ; \quad f(t) \geq 0$$

Standard solution:

$$\frac{dN(t)}{dt} = -f(t)N(t) \iff \frac{dN}{N} = d(\ln N) = -f(t)\,dt$$

$$\ln N(t) - \ln N(0) = -\int_0^t f(t')\,dt' \implies N(t) = \exp \left( -\int_0^t f(t')\,dt' \right)$$

$$F(t) = \int_0^t f(t')\,dt' \implies N(t) = \exp (-F(t) - F(0))$$

Assuming $F(\infty) = \infty$, i.e. always decay, sooner or later:

$$N(t) = R \implies t = F^{-1}(F(0) - \ln R)$$
Veto algorithm

What now if \( f(t) \) has no simple \( F(t) \) or \( F^{-1} \)?
Hit-and-miss not good enough, since for \( f(t) \leq g(t) \), \( g \) “nice”,

\[
t = G^{-1}(G(0) - \ln R) \implies N(t) = \exp \left( - \int_{0}^{t} g(t') \, dt' \right)
\]

\[
P(t) = -\frac{dN(t)}{dt} = g(t) \exp \left( - \int_{0}^{t} g(t') \, dt' \right)
\]

and hit-or-miss provides rejection factor \( f(t)/g(t) \), so that

\[
P(t) = f(t) \exp \left( - \int_{0}^{t} g(t') \, dt' \right)
\]

(modulo overall normalization), where it ought to have been

\[
P(t) = f(t) \exp \left( - \int_{0}^{t} f(t') \, dt' \right)
\]
The veto algorithm

1. start with $i = 0$ and $t_0 = 0$
2. $i = i + 1$
3. $t_i = G^{-1}(G(t_{i-1}) - \ln R)$, i.e. $t_i > t_{i-1}$
4. $y = Rg(t)$
5. while $y > f(t)$ cycle to 2

That is, when you fail, you keep on going from the time when you failed, and *do not* restart at time $t = 0$. (Memory!)
Study probability to have \( i \) intermediate failures before success:

Define \( S_g(t_a, t_b) = \exp \left( - \int_{t_a}^{t_b} g(t') \, dt' \right) \) ("Sudakov factor")

\[
P_0(t) = P(t = t_1) = g(t) \, S_g(0, t) \, \frac{f(t)}{g(t)} = f(t) \, S_g(0, t)
\]

\[
P_1(t) = P(t = t_2)
\]

\[
= \int_0^t dt_1 \, g(t_1) \, S_g(0, t_1) \left( 1 - \frac{f(t_1)}{g(t_1)} \right) g(t) \, S_g(t_1, t) \, \frac{f(t)}{g(t)}
\]

\[
= f(t) \, S_g(0, t) \, \int_0^t dt_1 \,(g(t_1) - f(t_1)) = P_0(t) \, I_{g-f}
\]

\[
P_2(t) = \cdots = P_0(t) \, \int_0^t dt_1 \,(g(t_1) - f(t_1)) \, \int_{t_1}^t dt_2 \,(g(t_2) - f(t_2))
\]

\[
= P_0(t) \, \int_0^t dt_1 \,(g(t_1) - f(t_1)) \, \int_0^t dt_2 \,(g(t_2) - f(t_2)) \, \theta(t_2 - t_1)
\]

\[
= P_0(t) \, \frac{1}{2} \left( \int_0^t dt_1 \,(g(t_1) - f(t_1)) \right)^2 = P_0(t) \, \frac{1}{2} \, I_{g-f}^2
\]
Veto algorithm

Generally, \( i \) intermediate times corresponds to \( i! \) equivalent ordering regions.

\[
P_i(t) = P_0(t) \frac{1}{i!} l_{g-f}^i
\]

\[
P(t) = \sum_{i=0}^{\infty} P_i(t) = P_0(t) \sum_{i=0}^{\infty} \frac{l_{g-f}^i}{i!} = P_0(t) \exp(l_{g-f})
\]

\[
= f(t) \exp \left( - \int_0^t g(t') \, dt' \right) \exp \left( \int_0^t (g(t') - f(t')) \, dt' \right)
\]

\[
= f(t) \exp \left( - \int_0^t f(t') \, dt' \right)
\]
MC methods summary

▶ Why? Very efficient when we have large n dimensional integrals and complex boundaries of integration ⇔ Many particles and complicated cuts.
▶ How?
  ▶ Formally, the Monte Carlo method is based on two basic theorems of the mathematical statistics: the Law of Large Numbers and the Central Limit Theorem.
  ▶ Pick a point at random according to a probability distribution:
    ▶ Inverse transform. Limitation: we need to know $F^{-1}$.
    ▶ If we don’t know $F^1$ - Hit and miss more efficient version of it importance sampling
    ▶ Branching algorithm
    ▶ Memory - Veto algorithm
Parton Shower and hard process
The hard subprocess, by definition, involves large momentum transfers and therefore the partons involved in it are violently accelerated.

The accelerated coloured partons will emit QCD radiation in the form of gluons leading to parton showers.

In principle, the showers represent higher-order corrections to the hard subprocess. However, it is not feasible to calculate these corrections exactly. Instead, an approximation scheme is used, in which the dominant contributions are included in each order.

These dominant contributions are associated with collinear parton splitting or soft (low-energy) gluon emission.

The conventional parton-shower formalism is based on collinear factorization.
Parton Shower and hard process

- Exact
- Approximate

jet-jet correlations
inner jet structure

S. Höche©
The hadronic cross section is

$$d\sigma(pp \rightarrow \mu^+ \mu^- g + X) = dx dx_b f(x, t)f_b(x_b, t)d\hat{\sigma} \quad , \quad d\hat{\sigma} = \frac{\left|\mathcal{M}(u\bar{u} \rightarrow \mu^+ \mu^- g)\right|^2 d\Phi_{n+1}}{4\sqrt{(pp_b)^2}}$$

S. Prestel©
\[ E_{(p-k)} \approx z E_p \] and small gluon \( p_\perp \) \( \Rightarrow \) Interal quark almost on-shell. Then:

\[ \frac{i(p' - k)}{(p - k)^2} \approx \frac{u(p_a)\bar{u}(p_a)}{p_a^2}, \quad d\Phi_{n+1} \approx d\Phi_n \frac{d\phi d\zeta dp_\perp^2}{4(2\pi)^3 (1 - z)}, \quad \frac{1}{4 \sqrt{(pp_b)^2}} \approx \frac{z}{4 \sqrt{(p_ap_b)^2}} \]

\[ \rightarrow \text{Matrix element, phase space integration and flux factors factorise!} \]

S. Prestel©
Parton Shower - outline

1. $e^+ e^- \text{ annihilation to jets}$
2. Universality of collinear emission
3. Sudakov form factors
4. Universality of soft emission
5. Angular ordering
6. Dipole cascades
PS is process-independent, however let's start with a simple example:
(see also Tutorial 1)

- Consider $e^+e^- \rightarrow 3$ partons

\[
\frac{1}{\sigma_{2 \rightarrow 3}} \frac{d\sigma_{2 \rightarrow 3}}{d \cos \theta dz} \sim C_F \frac{\alpha_s}{2\pi} \frac{2}{\sin^2 \theta} \frac{1 + (1 - z)^2}{z}
\]

- $\theta$ - angle of gluon emission
- $z$ - fractional energy of gluon

- Divergent in
  - Collinear limit: $\theta \rightarrow 0, \pi$
  - Soft limit: $z \rightarrow 0$

- Separate into two independent jets

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

- Independent jet evolution

\[
d\sigma_3 \sim \sigma_2 \sum_{\text{jets}} C_F \frac{\alpha_s}{2\pi} \frac{d\theta^2}{\theta^2} dz \frac{1 + (1 - z)^2}{z}
\]

It starts to look like we can iterate it!
Universality of collinear emission

- Same equation for any variable with same limiting behavior
  - Transverse momentum \( k_T^2 = z^2(1-z)^2\theta^2E^2 \)
  - Virtuality \( t = z(1-z)\theta^2E^2 \)

- Call this the “evolution variable”

\[
\frac{d\theta^2}{\theta^2} = \frac{dk_T^2}{k_T^2} = \frac{dt}{t} \quad \leftrightarrow \quad \text{collinear divergence}
\]

- Absorb \( z \)-dependence into flavor-dependent splitting kernel \( P_{ab}(z) \)

- Universal DGLAP evolution equation emerges

\[
d\sigma_{n+1} \sim \sigma_n \sum_{\text{jets}} \frac{dt}{t} \int dz \frac{\alpha_s}{2\pi} P_{ab}(z)
\]

We know where the divergence comes from and that it is universal, but not how to tame it!
What is a parton?

- Collinear parton pair $\iff$ single parton
- Introduce resolution criterion, e.g. $k_T > Q_0$
- Combine virtual contributions with unresolvable emissions: Cancels infrared divergences (Kinoshita-Lee-Nauenberg, Bloch-Nordsieck theorems)

- Instead of calculating it use the Unitary:

$$P(\text{resolved}) + P(\text{unresolved}) = 1$$
Sudakov form factor

Probability (emission between $q^2$ and $q^2 + dq^2$):

$$dP = \frac{\alpha_s}{2\pi} \int_{Q_0/q^2}^{1 - Q_0/q^2} dzP(z) \equiv \frac{dq^2}{q^2} \bar{P}(q^2)$$

Define probability (no emission between $Q^2$ and $q^2$) to be $\Delta(Q^2, q^2)$. We have evolution equation:

$$\frac{d\Delta(Q^2, q^2)}{dq^2} = \Delta(Q^2, q^2)dq^2 \frac{dP}{dq^2}$$

$$\Delta(Q^2, q^2) = \exp - \int_{q^2}^{Q^2} \frac{dk}{k} \bar{P}(k^2)$$

We know how to deal with it $\leftrightarrow$ Veto algorithm!

$$\Delta(Q^2, q^2) \equiv \Delta(Q^2)$$

Sudakov form factor = Probability (emitting no resolvable radiation)

$$\Delta(Q^2) \sim \exp - C_F \frac{\alpha_s}{2\pi} \log^2 \frac{Q^2}{Q_0^2}$$
Apart from collinear divergence, there is also a soft divergence: Also universal. But at amplitude level...

Soft gluon comes from everywhere in event → Quantum interference Spoils independent evolution picture? NO!

Outside angular ordered cones, soft gluons sum coherently: only see colour charge of whole jet. Angular ordering!
The differential cross section for $e^+e^- \rightarrow q\bar{q}g$ expressed in terms of the QCD "antenna" radiation pattern

$$d\sigma_3 = d\sigma_2 \frac{d\nu}{w} \frac{d\Omega}{2\pi} C_F W_{q\bar{q}}^g,$$

where

$$W_{q\bar{q}} = \frac{1 - \cos \theta_{q\bar{q}}}{(1 - \cos \theta_{qg})(1 - \cos \theta_{\bar{q}g})}.$$

QM interference between gluon emission off quark! How can soft emissions be independent??

We can split the antenna $W_{q\bar{q}}$ into two parts, $W_{q\bar{q}}^{(q)}$ and $W_{q\bar{q}}^{(\bar{q})}$, which are divergent only if the gluon is collinear to the quark / antiquark:

$$W_{q\bar{q}} = W_{q\bar{q}}^{(q)} + W_{q\bar{q}}^{(\bar{q})}, \quad \text{where} \quad W_{q\bar{q}}^{(q)} = \frac{1}{2} \left( W_{q\bar{q}} + \frac{1}{1 - \cos \theta_{qg}} - \frac{1}{1 - \cos \theta_{\bar{q}g}} \right).$$

Upon azimuthal integration, we obtain:

$$\frac{d\phi_{qg}}{2\pi} W_{q\bar{q}}^{(q)} = \begin{cases} 
1 & \text{if } \theta_{qg} < \theta_{q\bar{q}} \\
\frac{1}{1 - \cos \theta_{qg}} & \text{else}
\end{cases}.$$

That's angular ordering! Soft emissions are independent if ordered in emission angle!
Radiation from parton $i$ is bound to a cone, given by the colour partner parton $j$.

Results in angular ordered parton shower and suppresses soft gluons viz. hadrons in a jet.
Events with 2 hard (> 100 GeV) jets and a soft 3rd jet (∼ 10 GeV)

FIG. 13. Observed $\eta_3$ distribution compared to the predictions of (a) HERWIG; (b) ISAJET; (c) PYTHIA; (d) PYTHIA+.  

Best description with angular ordering.
Initial state parton shower

In principle identical to final state (for not too small $x$)
In practice different because both ends of evolution fixed:

Problem: Forward evolution not very efficient.
Solution: Backward evolution.
Formulate as backward evolution: start from hard scattering and work down in $q^2$, up in $x$ towards incoming hadron.
Algorithm identical to final state with $\Delta_i(Q^2, q^2)$ replaced by $\Delta_i(Q^2, q^2)/f_i(x, q^2)$
Parton Shower - Not at all unique!

Some (more or less clever) choices still to be made. **Standard shower** language of $a \rightarrow bc$ successive branchings

- $q$ evolution variable can be $\theta$ (Herwig), $Q^2$ (old Pythia), $p_\perp$, ...
- Choice of $q_{\text{min}}$ scale not fixed.
- Integration limits, available parton shower phase space.
- Massless partons become massive. How?
- Initial-state showers to increase the Monte Carlo efficiency the backward evolution is used.

**Dipole shower**: dipole splitting is a $2 \rightarrow 3$

In this framework one can get the correct logarithmic structure for both soft and collinear emissions without angular-ordering requirement. First ARIADNE, now also available in SHERPA, Herwig++, VINCIA.
Dipole Shower

In the soft limit, we found:

\[
\frac{d\sigma_{n+1}}{d\sigma_n} = \int \frac{dw}{w} \frac{d\Omega}{2\pi} C_F \sum_{ij} W_{ij}, \quad \text{where} \quad W_{q\bar{q}} = \frac{1 - \cos \theta_{q\bar{q}}}{(1 - \cos \theta_{qg})(1 - \cos \theta_{\bar{q}g})}.
\]

We could have directly used \( W_{ij} \) as splitting probability (QCD antenna), or partitioned cleverly (QCD dipole).

\[
\frac{p_ip_k}{(p_ip_j)(p_jp_k)} \rightarrow \frac{1}{p_ip_j} \frac{p_ip_k}{(p_i + p_k)p_j} + \frac{1}{p_kp_j} \frac{p_ip_k}{(p_i + p_k)p_j}.
\]

In a parton shower, they are mostly used in their spin-averaged form, which reads

\[
\langle V \rangle_{qg}(\bar{z}, y) = C_F \left[ \frac{2}{1 - \bar{z}(1 - y)} - (1 + \bar{z}) \right],
\]

\[
\langle V \rangle_{gg}(\bar{z}, y) = 2CA \left[ \frac{1}{1 - \bar{z}(1 - y)} + \frac{1}{1 - (1 - \bar{z})(1 - y)} - 2 + \bar{z}(1 - \bar{z}) \right].
\]

See Tutorial 1. Two advantages over 1->2 parton showers

a) The soft limit of QCD is described in a more natural way, and

b) Momentum conservation is simpler (recoil particle).
Parton Shower: Initial State:


**Drell-Yan $p_T$ Spectrum (at $Q=M_Z$)**

\[ p_{\perp} (Z) \sim \sum_{j \in jets} p_{\perp} (j) \]

**Particularly sensitive to**

1. $\alpha_s$ renormalization scale choice
2. Recoil strategy (color dipoles vs global vs …)
3. FSR off ISR (ISR jet broadening)

Non-trivial result that modern GPMC shower models all reproduce it $\sim$ correctly

*Note: old PYTHIA 6 model (Tune A) did not give correct distribution, except with extreme $\mu_R$ choice (DW, D6, Pro-Q20)*
Parton Shower: Final State

**Integrated Jet Shape as function of R**
- Central Region $|\gamma| < 0.3$
- $80 < p_T < 110$

**Integrated Jet Shape as function of R**
- Forward $2.1 < |\gamma| < 2.8$
- $80 < p_T < 110$

**Ratio to ATLAS**
- **Central region OK**
  - Also ok for smaller $p_T$ values only if UE is well tuned

**Ratio to ATLAS**
- **Forward region less good**
  - (Also larger UE uncertainties)
Jet pruning/filtering designed to isolate new physics through hard internal jet structure but also a good probe of final state parton shower.

[CMS-PAS-JME-10-013]

Leading jet pruned jet mass and "mass drop" (ratio of masses of highest $p_T$ subjet to full jet)
One example: “Non-perturbative gluon emission model”

Primordial $k_T$ from soft, non-perturbative gluons

Allow for very soft gluon radiation (all cutoffs, masses $\to \epsilon$).

Get good description of DY $p_T$ spectrum (38.8, 62 and 1800 GeV) using only small Gaussian primordial $k_T \sim 0.4$ GeV , (allowed by Heisenberg), not $>2$ GeV.

"...A detailed study of the jet properties reveals that quark- and gluon-jets look more similar to each other in the data than in the Pythia 6 simulation and less similar than in the Herwig++ simulation. As a result, the ability of the tagger to reject gluons at a fixed quark efficiency is up to a factor of two better in Pythia 6 and up to 50% worse in Herwig++ than in data..."
Parton shower - developments

Herwig 7
- New parton shower variables in Herwig++ (still angular-ordered).
- Dipole shower, based upon Catani-Seymour dipoles.

Sherpa
- Catani-Seymour Shower default by now, also matched via CKKW (see later). **New shower: DIRE**

Pythia 8
- $p_\perp$ ordered shower based on dipole showering. VINCIA (plugin), **New shower: DIRE (plugin)**
- Interleaved with Multiple partonic interactions.

IR Safe Summary (ISR/FSR):
- LO showers generally in good $O(20\%)$ agreement with LHC (modulo bad tunes, pathological cases)
- Room for improvement: Quantification of uncertainties is still more art than science. **Recent progress by all generators.**
- Bottom Line: perturbation theory is solvable. Expect progress for example: NLO Parton Shower - Cracow group S. Jadach at al., S. Prestel and S. Höche, P. Skands ...
Parton-shower uncertainties - example Herwig 7


Two Parton Showers:
- Angular-ordered Parton Shower (PS)
- $p_T$-ordered Dipole Shower

Up/Down Variations of:
- $\mu_H$ - argument of PDF, $\alpha_S$ in hard matrix element
- $\mu_S$ - argument of PDF, $\alpha_S$ in the shower
- $\mu_Q$ - shower starting/veto scale
- $\mu_{IR}$ - shower cutoff
Run-time improvement via parton-shower reweighting

[Bellm, Platzer, Richardson, AS, Webster, Phys.Rev. D94 (2016)]

Transverse momentum of Higgs boson in $pp \rightarrow gg \rightarrow H$, $\sqrt{S} = 13$ TeV

- excellent agreement between individual runs for different scales and reweighting
- significant speed improvements: time in seconds for 10 000 events

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>AO</td>
<td>Off</td>
<td>79.8</td>
<td>94.2</td>
<td>-0.18</td>
<td>384.4</td>
<td>249.1</td>
<td>0.35</td>
<td>416.7</td>
<td>375.1</td>
<td>0.09</td>
<td></td>
</tr>
<tr>
<td></td>
<td>On</td>
<td>183.2</td>
<td>128.3</td>
<td>0.30</td>
<td>738.7</td>
<td>364.3</td>
<td>0.51</td>
<td>751.4</td>
<td>482.3</td>
<td>0.35</td>
<td></td>
</tr>
<tr>
<td>Dipole</td>
<td>Off</td>
<td>99.6</td>
<td>52.8</td>
<td>0.47</td>
<td>435.4</td>
<td>161.9</td>
<td>0.63</td>
<td>462.7</td>
<td>213.6</td>
<td>0.54</td>
<td></td>
</tr>
<tr>
<td></td>
<td>On</td>
<td>271.8</td>
<td>108.2</td>
<td>0.60</td>
<td>831.7</td>
<td>286.6</td>
<td>0.65</td>
<td>859.2</td>
<td>340.1</td>
<td>0.60</td>
<td></td>
</tr>
</tbody>
</table>
In order to provide fully exclusive modeling of high-energy collisions we have to solve multidimensional integrals (many particles) - MC methods very efficient!

Accelerated colour charges radiate gluons. Gluons are also charged → Parton Shower cascade

Modern parton shower models are very sophisticated implementations of perturbative QCD

but would be useless without hadronization models...
Thank you for your attention!
PS veto algorithm in details

- Start with set of \( n \) partons at scale \( t' \), which evolve collectively Sudakov form factors factorize, schematically

\[
\Delta(t, t') = \prod_{i=1}^{n} \Delta_i(t, t') \\
\Delta_i(t, t') = \prod_{j=q, g} \Delta_{i \rightarrow j}(t, t')
\]

- Use veto algorithm to find new scale \( t \) where branching occurs
  - Generate \( t \) using overestimate \( \alpha_s^{\text{max}} P_{ab}^{\text{max}}(z) \)
  - Determine “winner” parton \( i \) and select new flavor \( j \)
  - Select splitting variable according to overestimate
  - Accept point with weight \( \alpha_s(k_T^2)P_{ab}(z)/\alpha_s^{\text{max}} P_{ab}^{\text{max}}(z) \)

- Construct splitting kinematics and update color flow

- Continue until \( t < t_c \)
Backward evolution