Monte Carlo Techniques and Event Generation Lecture 1: Introduction to Monte Carlo Techniques

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Terascale Monte Carlo School DESY Hamburg, April 13-17 2015

Introduction

- In classical and quantum electrodynamics accelerated charges radiate.
- Similarly in QCD accelerated colour charges radiate.
- This gives a cascade of quarks and gluons, the parton shower



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Plan

- Infrared divergences.
- Colinear Emission.
- Sudakov Form Factors.
- Soft emission and colour coherence.
- Initial-State radiation.
- Heavy quarks.
- Dipole cascades.
- Intrinsic p_{\perp}

Gluon Emission

The total cross section is

$$\sigma(e^+e^- o q\bar{q}g) = \sigma_0 C_F rac{lpha_S}{2\pi} \int \mathrm{d}x_1 \mathrm{d}x_2 rac{x_1^2 + x_2^2}{(1-x_1)(1-x_2)},$$

where $x_i \equiv 2p_i/\sqrt{s}$ and $\sigma_0 = \sigma(e^+e^- \rightarrow q\bar{q})$.

■ Divergent at the edge of phase space as x_{1,2} → 1 so that the total cross section is σ = ∞!

Gluon Emission

- Common feature of all perturbative QCD calculations.
- Configurations which are indistinguishable from the leading-order result are divergent.
- Physically there are two regions where this happens
 1 Colinear limit: x₁ → 1 at fixed x₂ or x₂ → 1 at fixed x₁

$$2p_2 \cdot k = \frac{sx_2x_3}{2}(1 - \cos \theta_{23}) = s(1 - x_1) \implies (1 - \cos \theta_{23}) = \frac{2(1 - x_1)}{x_2x_3} \to 0.$$

2 Soft limit: $x_{1,2} \rightarrow 1$ at fixed $\frac{1-x_1}{1-x_2}$

$$E_g = rac{\sqrt{s}}{2} x_3 = rac{\sqrt{s}}{2} (1 - x_1 + 1 - x_2) o 0.$$

Both universal features of QCD matrix elements.

Colinear Limit

If we take k parallel to p_2 ($\theta_{23} = 0$) we can define

$$p_2 = (1-z)\bar{p}_2, \qquad k = z\bar{p}_2, \qquad \text{with} \ \bar{p}_2^2 = 0.$$

In this limit the matrix element factorizes

$$|\mathcal{M}_{q\bar{q}g}|^2 = |\mathcal{M}_{q\bar{q}}|^2 imes rac{g_s^2}{p_2 \cdot k} imes C_F rac{1+(1-z)^2}{z}.$$

As does the phase space

$$\mathrm{d}x_1\mathrm{d}x_2 \longrightarrow \frac{1}{4}z(1-z)\mathrm{d}z\mathrm{d}\theta_{23}^2.$$

Colinear Limit

Putting this together

$$\sigma = \sigma_0 \int \frac{\mathrm{d}\theta_{23}^2}{\theta_{23}^2} dz C_F \frac{\alpha_S}{2\pi} \frac{1 + (1 - z)^2}{z}$$

- The Dokshitzer-Gribov-Lipatov-Altarelli-Parisi splitting function is a universal probability distribution for the radiation of a colinear gluon in any process producing a quark.
- Exactly same form for anything proportional to θ^2 , e.g.
 - transverse momentum $k_{\perp}^2 = z^2(1-z)^2\theta^2$;
 - invariant mass $q^2 = z(1-z)\theta^2 E^2$.

such that

$$\frac{\mathrm{d}\theta^2}{\theta^2} = \frac{\mathrm{d}k_{\perp}^2}{k_{\perp}^2} = \frac{\mathrm{d}q^2}{q^2}$$

Parton Shower

The simulation of QCD radiation is based this factorization, *i.e*

$$\mathrm{d}\sigma_{n+1} = \mathrm{d}\sigma_n \frac{\mathrm{d}\theta^2}{\theta^2} \mathrm{d}z \frac{\alpha_S}{2\pi} P_{ji}(z)$$

where the splitting function only depends on the spin and flavour of the partons.



Splitting Functions



Parton Shower

- This expression is singular as $\theta \to 0$.
- What is a parton? (or what is the difference between a colinear pair and a parton).
- Introduce a resolution criterion, e.g. $k_{\perp} > Q_0$.
- Combine the virtual corrections and unresolvable emission



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Unresolvable Emission Infinite

 "Unitarity": Unresolved + Resolved =1. Obviously not the full perturbative information. Defines the virtual contributions to allow for a probabilistic interpretation of emissions.
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Sudakov Form Factor

We can then exponentiate the real emission piece

$$\begin{aligned} \mathcal{P}(\text{unresolved}) &= 1 - \mathcal{P}(\text{resolved}), \\ &= 1 - \int_{q^2}^{Q^2} \frac{\mathrm{d}k^2}{k^2} \int_{\frac{Q_0^2}{q^2}}^{1 - \frac{Q_0^2}{q^2}} \mathrm{d}z \frac{\alpha_S}{2\pi} P(z), \\ &= \exp\left(-\int_{q^2}^{Q^2} \frac{\mathrm{d}k^2}{k^2} \int_{\frac{Q_0^2}{q^2}}^{1 - \frac{Q_0^2}{q^2}} \mathrm{d}z \frac{\alpha_S}{2\pi} P(z)\right). \end{aligned}$$

- The Sudakov form factor which is the probability of evolving between two scales and emitting no radiation.
- More strictly it is the probability of evolving from a high scale to the cut-off with no resolvable emission.

Sudakov Form Factor

More formally, the probability of emission between $\mathrm{d}q^2$ and $q^2 + \mathrm{d}q^2$ is

$$\mathrm{d}\mathcal{P} = \frac{\mathrm{d}q^2}{q^2} \int_{\frac{Q_0^2}{q^2}}^{1-\frac{Q_0^2}{q^2}} \mathrm{d}z \frac{\alpha_S}{2\pi} P(z)$$

We can then write a differential equation for the evolution of the probability of no-emission between Q² and q², Δ(Q², q²)

$$\mathrm{d}\Delta(Q^2,q^2) = \Delta(Q^2,q^2)\mathrm{d}\mathcal{P} \ \Rightarrow \ \frac{\mathrm{d}\Delta(Q^2,q^2)}{\Delta(Q^2,q^2)} = \frac{\mathrm{d}q^2}{q^2} \int_{\frac{Q_0^2}{q^2}}^{1-\frac{Q_0^2}{q^2}} \mathrm{d}z \frac{\alpha_S}{2\pi} P(z)$$

giving

$$\Delta(Q^2,q^2) = \exp\left(-\int_{q^2}^{Q^2} \frac{\mathrm{d}k^2}{k^2} \int_{\frac{Q_0^2}{q^2}}^{1-\frac{Q_0^2}{q^2}} \mathrm{d}z \frac{\alpha_s}{2\pi} P(z)\right)$$

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Numerical Procedure

Radioactive Decay

- Start with an isotope.
- Work out when it decays by generating a random number R∃[0, 1] and solving

$$R = \exp\left[-\frac{t}{\tau}\right],$$

where au is its lifetime.

- Generate another random number and use the branching ratios to find the decay mode.
- Generate the decay using the masses of the decay products and phase space.
- Repeat the process for any unstable decay products.
- This algorithm is actually used in Monte Carlo event generators to simulate particle decays.

Parton Shower

- Start with a parton at a high virtuality, Q, typical of the hard collision.
- Work out the scale of the next branching by generating a random number R∃[0, 1] and solving

$$R=\Delta(Q^2,q^2)$$

where q is the scale of the next branching.

- If there's no solution for $q > Q_0$ then stop.
- Otherwise workout the type of branching.
- Generate the momenta of the decay products using the splitting functions.
- Repeat the process for the partons produced in the branching.

Veto Algorithm

- Usually we cannot easily solve $\Delta(Q^2, q^2) = \mathcal{R}$.
- Instead we start by picking an overestimate $P_{over}(z) \ge P(z)$ which is easily invertible, *i.e.* we can calculate $H(z) = \int P_{over}(z) dz$ and $H^{-1}(z)$.
- Also overestimate of the integration region $z_{\min}^{\text{over}} \leq z_{\min}$ and $z_{\max}^{\text{over}} \geq z_{\max}$, and the maximum value of α_s , $\alpha_s^{\text{over}} \geq \alpha_s(p_{\perp}(q^2, z)) \forall z, q^2$.
- We now have an overestimate of the integrand of the Sudakov form factor, *i.e.*

$$F(k^2) = \frac{1}{k^2} \int_{z_{\min}}^{z_{\max}} \mathrm{d}z \frac{\alpha_S}{2\pi} P(z) \quad \to \quad G(k^2) = \frac{1}{k^2} \int_{z_{\min}^{\mathrm{over}}}^{z_{\max}^{\mathrm{over}}} \mathrm{d}z \frac{\alpha_S^{\mathrm{over}}}{2\pi} P_{\mathrm{over}}(z)$$

Veto Algorithm

• We can solve this to get a first trial value of q^2

$$\ln \mathcal{R} = -\int_{q^2}^{Q^2} \frac{\mathrm{d}k^2}{k^2} \int_{z_{\min}^{\text{over}}}^{z_{\max}^{\text{over}}} \mathrm{d}z \frac{\alpha_{S}^{\text{over}}}{2\pi} P_{\text{over}}(z) \Rightarrow q^2 = Q^2 \exp\left(\frac{\ln \mathcal{R}}{\int_{z_{\min}^{\text{over}}}^{z_{\max}^{\text{over}}} \mathrm{d}z \frac{\alpha_{S}^{\text{over}}}{2\pi} P_{\text{over}}(z)}\right)$$

- However we cannot do simple accept/reject
- Instead generate a value of z using

$$z = H^{-1} \left[H(z_{\min}^{\mathrm{over}}) + \mathcal{R}(H(z_{\max}^{\mathrm{over}}) - H(z_{\min}^{\mathrm{over}}))
ight]$$

We reject the emission if z is outside the true limits or with probability

$$rac{F(q^2)}{G(q^2)} = rac{rac{lpha_S}{2\pi}P(z)}{rac{lpha^{
m over}}{2\pi}P_{
m over}(z)} \geq \mathcal{R}$$

if z is inside the true limits but if the try is rejected start again with $Q^2 = q^2$ and generate another try.

Veto Algorithm

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If we define $\mathcal{P}_n(q^2)$ to be probability we accept q^2 after rejecting n attempts then the probability of generating q^2 is $\sum_{n=0}^{\infty} \mathcal{P}_n(t)$, where

$$\begin{split} \mathcal{P}_{0}(q^{2}) &= G(q^{2})\Delta^{\text{over}}(Q^{2},q^{2})\frac{F(q^{2})}{G(q^{2})} = \Delta^{\text{over}}(Q^{2},q^{2})F(q^{2})\\ \mathcal{P}_{1}(q^{2}) &= \int_{q'^{2}}^{Q^{2}} \mathrm{d}q'^{2}G(q'^{2})\Delta^{\text{over}}(Q^{2},q'^{2}) \left[1 - \frac{F(q'^{2})}{G(q'^{2})}\right]G(q^{2})\Delta^{\text{over}}(q'^{2},q^{2})\frac{F(q^{2})}{G(q^{2})}\\ &= F(q^{2})\Delta^{\text{over}}(Q^{2},q^{2})\int_{q^{2}}^{Q^{2}} \mathrm{d}q'^{2}\left(G(q'^{2}) - F(q'^{2})\right) \end{split}$$

$$\mathcal{P}_n(q^2) = \frac{1}{n!} F(q^2) \Delta^{\text{over}}(Q^2, q^2) \left[\int_{q^2}^{Q^2} \mathrm{d}q'^2 \left(G(q'^2) - F(q'^2) \right) \right]^n$$

Veto Algorithm

Summing

$$\begin{split} \sum_{n=0}^{\infty} \mathcal{P}_n(t) &= F(q^2) \Delta^{\text{over}}(Q^2, q^2) \sum_{n=0}^{\infty} \left[\int_{q^2}^{Q^2} \mathrm{d}q'^2 \left(G(q'^2) - F(q'^2) \right) \right]^n \\ &= F(q^2) \Delta^{\text{over}}(Q^2, q^2) \exp\left[\int_{q^2}^{Q^2} \mathrm{d}q'^2 \left(G(q'^2) - F(q'^2) \right) \right] \\ &= F(q^2) \exp\left[- \int_{q^2}^{Q^2} \mathrm{d}q'^2 G(q'^2) \right] \exp\left[\int_{q^2}^{Q^2} \mathrm{d}q'^2 \left(G(q'^2) - F(q'^2) \right) \right] \\ &= F(q^2) \Delta^{\text{over}}(Q^2, q^2) \end{split}$$

as required.

Monte Carlo Procedure

The key difference between the different Monte Carlo simulations is in the choice of the evolution variable.

Evolution Scale

- Virtuality, q^2
- **Transverse Momentum**, k_{\perp}
- Angle, θ
- Energy fraction, z
 - Energy fraction
 - Light-cone momentum fraction
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Are all the same in the colinear limit.

Soft Emission

- We have only considered colinear emission. What about soft emission?
- Soft gluons come from all over the event.
- There is quantum interference
- Does this spoil the parton shower picture?



Soft Limit

In the limit that $E_g
ightarrow 0$ the matrix element for the $e^+e^-
ightarrow q ar{g}$ factorizes

$$\mathcal{M}_{q\bar{q}g} = \mathcal{M}_{q\bar{q}}g_s t^a_{ij}\left(rac{p_1}{p_1\cdot k} - rac{p_2}{p_2\cdot k}
ight)\cdot\epsilon_A(k).$$

- Called the Eikonal Current.
- The matrix element squared therefore factorizes in this case

$$|\mathcal{M}_{q\bar{q}g}|^2 = |\mathcal{M}_{q\bar{q}}|^2 g_s^2 C_F \frac{2p_1 \cdot p_2}{p_1 \cdot kp_2 \cdot k}.$$

In this case the phase space is

$$\mathrm{d} x_1 \mathrm{d} x_2 \longrightarrow \frac{2}{s} E_g \mathrm{d} E_g \mathrm{d} \cos \theta.$$

Soft Limit

So in the soft limit

$$\sigma = \sigma_0 \int C_F \frac{\alpha_S}{2\pi} \frac{\mathrm{d}E_g}{E_g} \mathrm{d}\cos\theta \frac{2(1-\cos\theta_{qq})}{(1-\cos\theta_{qg})(1-\cos\theta_{qg})}.$$

- Gives the Dipole Radiation pattern.
- Universal probability distribution to emit a soft gluon from any colour-connected pair of partons.
- Only universal at the amplitude level

Angular Ordering

- In the soft limit the matrix element factorizes but at the amplitude level.
- The remarkable result is that if we take the large number of colours limit much of the interference is destructive.
- In particular if we consider the colour flow in an event.
- QCD radiation only occurs in a cone up to the direction of the colour partner.
- The best choice of evolution variable is therefore an angular one



Colour Coherence



- Wide angle soft gluons cannot resolve the difference between a gluon and "colinear" quark and gluon with the same quantum numbers.
- Called Colour Coherence
- Angular ordering is one way of including this physics, but there are others.

Accuracy of Parton Shower simulations

Formally the parton shower is accurate to leading log.

$$\Delta(Q^2, Q_0^2) pprox \exp\left[-C_F rac{lpha_S}{2\pi} \ln^2\left(rac{Q^2}{Q_0^2}
ight)
ight]$$

- However Monte Carlo simulations include a number of subleading effects.
- The most important is the conservation of energy and momentum.
- Others include the choice of the scale for α_S .

Running Coupling

Some of the higher order effects are included by

replacing $\alpha_S \rightarrow \alpha_S(k_\perp^2)$

- Gives more emission as $k^2 \rightarrow Q_0^2$. The phase space fills with soft gluons.
- Must avoid the Landau pole $K_{\perp}^2 \gg \Lambda^2$ so that Q_0^2 becomes a physical parameter.

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LEP Event Shapes



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LEP Jet Resolution



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Jet Shapes



Phys. Rev. D83 052003 ATLAS (2011)

Hadron-Hadron Simulations

- In order to simulate hadron collisions we also need to simulate initial-state radiation.
- In principle this is similar to final-state radiation, but in practice there is a complication.
- For final-state radiation: One end of the evolution fixed, the scale of the hard collision.
- For initial-state radiation: Both ends of the evolution fixed, the hard collision and the incoming hadron.



Use a different approach based on the evolution equations.

Initial-State Radiation

There are two options for the initial-state shower:

- Forward Evolution
 - Start at the hadron with the distribution of partons given by the PDF.
 - Use the parton shower to evolve to the hard collision.
 - Reproduces the PDF by a Monte Carlo procedure.
 - Unlikely to give an interesting event at the end, so highly inefficient.
- Backward Evolution
 - Start at the hard collision and evolve backwards to the proton guided by the PDF.
 - Much more efficient in practice.

Initial-State Radiation

The evolution equation for the PDF can be written as

$$t\frac{\mathrm{d}f_b(x,Q^2)}{\mathrm{d}t} = \sum_{a} \int_x^1 \frac{\mathrm{d}z}{z} f_a\left(\frac{x}{z},Q^2\right) \frac{\alpha_s}{2\pi} P_{a\to bc}(z) \quad \text{where} \quad t = \ln\left(\frac{Q^2}{\Lambda^2}\right)$$

$$\frac{\mathrm{d}f_b(x,Q^2)}{f_b(x,Q^2)} = \frac{\mathrm{d}t}{t} \sum_a \int_x^1 \frac{\mathrm{d}z}{z} \frac{x'f_a\left(x',Q^2\right)}{xf_b(x,Q^2)} \frac{\alpha_S}{2\pi} P_{a \to bc}(z) \quad \text{where} \quad x' = \frac{x}{z}$$

This can be written as a Sudakov form-factor for evolving backwards in time, i.e from the hard collision at high Q² to lower with

$$\Delta = \exp\left(-\frac{\mathrm{d}t}{t}\sum_{a}\int_{x}^{1}\frac{\mathrm{d}z}{z}\frac{x'f_{a}\left(x',Q^{2}\right)}{xf_{b}(x,Q^{2})}\frac{\alpha_{S}}{2\pi}P_{a\to bc}(z)\right).$$

Backward Evolution

- The evolution equations give the PDFs at (x, Q²) as a function of those at (> x, < Q²)
- Backward evolution starts from the hard scattering at (x, Q²) and work ↓ q² and ↑ x towards the incoming hadron.



Hadron Collisions

- The hard scattering sets up the initial conditions for the parton shower.
- Colour coherence is important here too.
- Each parton can only emit in a cone stretching to its colour partner.



Essential to fit the Tevatron data.

Colour Coherence

- Distributions of the pseudorapidity of the third jet.
- At the time only described by HERWIG which has complete treatment of colour coherence.
- PYTHIA+ had partial.
- Modern generators now all include coherence in some manner.



PRD50, 5562, CDF (1994)

Colour Coherence



PRD50, 5562, CDF (1994)

Colour Coherence



CMS-PAS-SMP-12-010 CMS (2013)

Hadronic Event Shapes

- In hadron collisions we can't use the same event shapes as e^+e^- collisions due to radiation along the beam direction.
- There are however a range of event shapes using transverse quantities, for example

$$au_{\perp,\mathcal{C}} = 1 - \max_{\hat{n}_{\mathcal{T}}} rac{\sum_i |ec{p}_{\perp,i} \cdot \hat{n}_{\mathcal{T}}|}{\sum_i p_{\perp,i}}.$$

Hadronic Event Shapes



CMS Phys. Lett. B699 (2011) 48-67



Heavy Quarks

 The colinear singularity is regulated by the quark mass.

$$2p_2 \cdot k = 2E_g(E_q - |p_q| \cos \theta_{23})$$

= $2E_g|p_q|(\sqrt{1 + \frac{m^2}{|p_q|^2}} - \cos \theta_{23})$

- Taking the azimuthal average of the soft radiation function gives a smooth suppression of radiation as θ → 0 starting from θ ~ π/F.
- Historically implemented as a cut-off.



Heavy Quarks

Better treatment involves the use of the quasi-colinear splitting functions Catani et.al Phys.Lett. B500 149-160 (2001)

$$\mathrm{d}\mathcal{P} = \frac{\alpha_S}{2\pi} \frac{\mathrm{d}q^2}{q^2 - m^2} P_{\tilde{i}j \to ij}(z, q^2)$$

where

$$\begin{split} P_{q \to qg} &= \frac{C_F}{1-z} \left[1 + z^2 - \frac{2(1-z)m_q^2}{q^2 - m_q^2} \right], P_{g \to q\bar{q}} &= T_R \left[1 - 2z \left(1 - z \right) + \frac{2m_q^2}{q^2 - m_q^2} \right], \\ P_{\tilde{g} \to \tilde{g}g} &= \frac{C_A}{1-z} \left[1 + z^2 - \frac{2(1-z)m_{\tilde{g}}^2}{q^2 - m_{\tilde{g}}^2} \right], P_{\tilde{q} \to \tilde{q}g} &= \frac{2C_F}{1-z} \left[z - \frac{(1-z)m_{\tilde{q}}}{q^2 - m_{\tilde{q}}^2} \right]. \end{split}$$

• Gives a smooth suppression as $\theta \to 0$.

Heavy Quarks

- Only exact for either:
 - soft emission $E_{\text{gluon}} \rightarrow 0$;
 - radiation from scalars.
- In general the radiation depends on:
 - Gluon energy;
 - spins of radiating particles and colour partner;
 - colours of the particles;
 - *i.e.* process-dependent mass corrections.





Jet Shapes for bottom quark jets





arXiv:1307.5749 ATLAS (2013)

b-fragmentation function



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The Colour Dipole Model

- Conventional parton showers: start from colinear limit, modify to incorporate soft gluon coherence
- Colour Dipole Model: start from soft limit Emission of soft gluons from colour-anticolour dipole universal (and classical):

$$\mathrm{d}\sigma \sim \sigma_0 \frac{1}{2} C_A \frac{\alpha_{\mathcal{S}}(k_\perp)}{2\pi} \frac{\mathrm{d}k_\perp^2}{k_\perp^2} \mathrm{d}y,$$

where y = is the rapidity of the emitted particle.

After emitting a gluon, colour dipole is split:

The Colour Dipole Model

- Subsequent dipoles continue to split.
- Conventional parton-showers $1 \rightarrow 2$ parton splittings.
- **CDM** one dipole to two dipoles, $2 \rightarrow 3$ partons.
- Problems with the treatment of initial=-state radiation.
- The hadronic remnant forms a dipole with scattered quark.
- But as the remnant is an extended object there is a suppression.

Dipole Cascades

- Most new shower algorithms are based on a dipole picture.
- However most split the dipole into two pieces, one for radiation from each of the partons forming it, as in Catani-Seymour subtraction.
- The partner is used to absorb recoil and define the radiation pattern.

Dipole Vinica, ARIADNE

Split PYTHIA6.3, PYTHIA8, Sherpa and Herwig++ dipole showers

Primordial p_{\perp}

- The partons inside the proton have some motion with $p_{\perp} \sim \frac{1}{1 \text{ fm}}$.
- Intrinsic p_{\perp} is essential to describe the low p_{\perp} behaviour of Drell-Yan.
- Particularly important at the Tevatron as no perturbative radiation in some events.
- Less important at the LHC, pp and higher energy.



Primordial p_{\perp}



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Older Programs

PYTHIA 6: two showers

- q² ordering with veto of non-ordered final state emission and partial implementation of angular ordering in initial state;
- p_{\perp} -ordered parton showers, interleaved with multi-parton interactions and dipole-style recoil.

Matrix element for first emission in many processes and a large range of hard processes.

- HERWIG6: complete implementation of colour coherence; NLO evolution for large x; smaller range of hard processes.
- ARIADNE: complete implementation of colour dipole model; best fit to HERA data; interfaced to PYTHIA for hard processes.

Modern Programs

- PYTHIA8: new program with many of the same features as PYTHIA6, many obsolete features removed.
- SHERPA: new program built from scratch; either older q² or newer p_⊥-ordered dipole showers; multi-jet matching scheme (CKKW) and NLO built in.
- Herwig++: new program with similar parton shower to HERWIG (angular ordered) plus quasi-colinear limit and recoil strategy based on colour flow; spin correlations.



- Accelerated colour charges radiate gluons.
- As the gluon is also coloured this leads to a cascade of gluons.
- Modern parton shower algorithms are sophisticated implementations of perturbative QCD.
- Allows us to evolve from the scale of the hard collision to the hadronization scale.
- However we then need non-perturbative hadronization models.