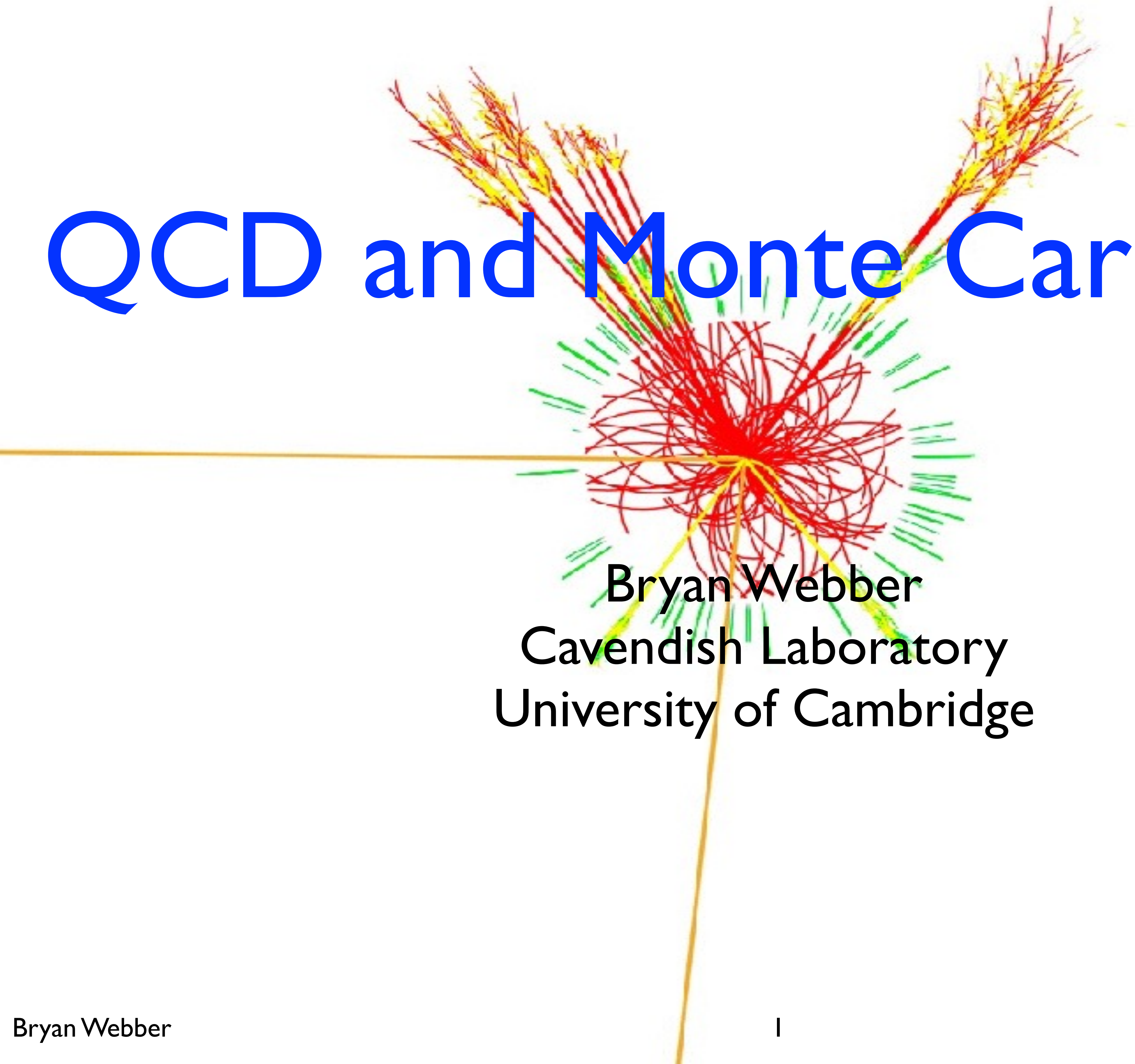
QCD and Monte Carlo Tools



Bryan Webber
Cavendish Laboratory
University of Cambridge

Monte Carlo Event Generation

- Aim is to produce simulated (particle-level) datasets like those from real collider events
  - i.e. lists of particle identities, momenta, ...
  - simulate quantum effects by (pseudo)random numbers
- Essential for:
  - Designing new experiments and data analyses
  - Correcting for detector and selection effects
  - Testing the SM and measuring its parameters
  - Estimating new signals and their backgrounds

Monte Carlo Basics

Monte Carlo Integration

- Basis of all Monte Carlo methods:

$$I = \int_a^b f(x)\,dx \approx \frac{1}{N}\sum_{i=1}^{N} \underbrace{(b-a)f(x_i)}_{\text{weight } w_i} \equiv I_N$$

where x_i are randomly (uniformly) distributed on [a,b].

- Then $I = \lim\limits_{N\to\infty} I_N = E[w]\;,\quad \sigma_I = \sqrt{\mathrm{Var}[w]/N}$

where $\mathrm{Var}[w] = E[(w-E[w])^2] = E[w^2] - (E[w])^2$

$$= (b-a)\int_a^b [f(x)]^2 dx - [\int_a^b f(x)\,dx]^2 \equiv V$$

$$\boxed{I = I_N \pm \sqrt{V/N}}$$

Central limit theorem:
$P(< 1\sigma) = 68\%$

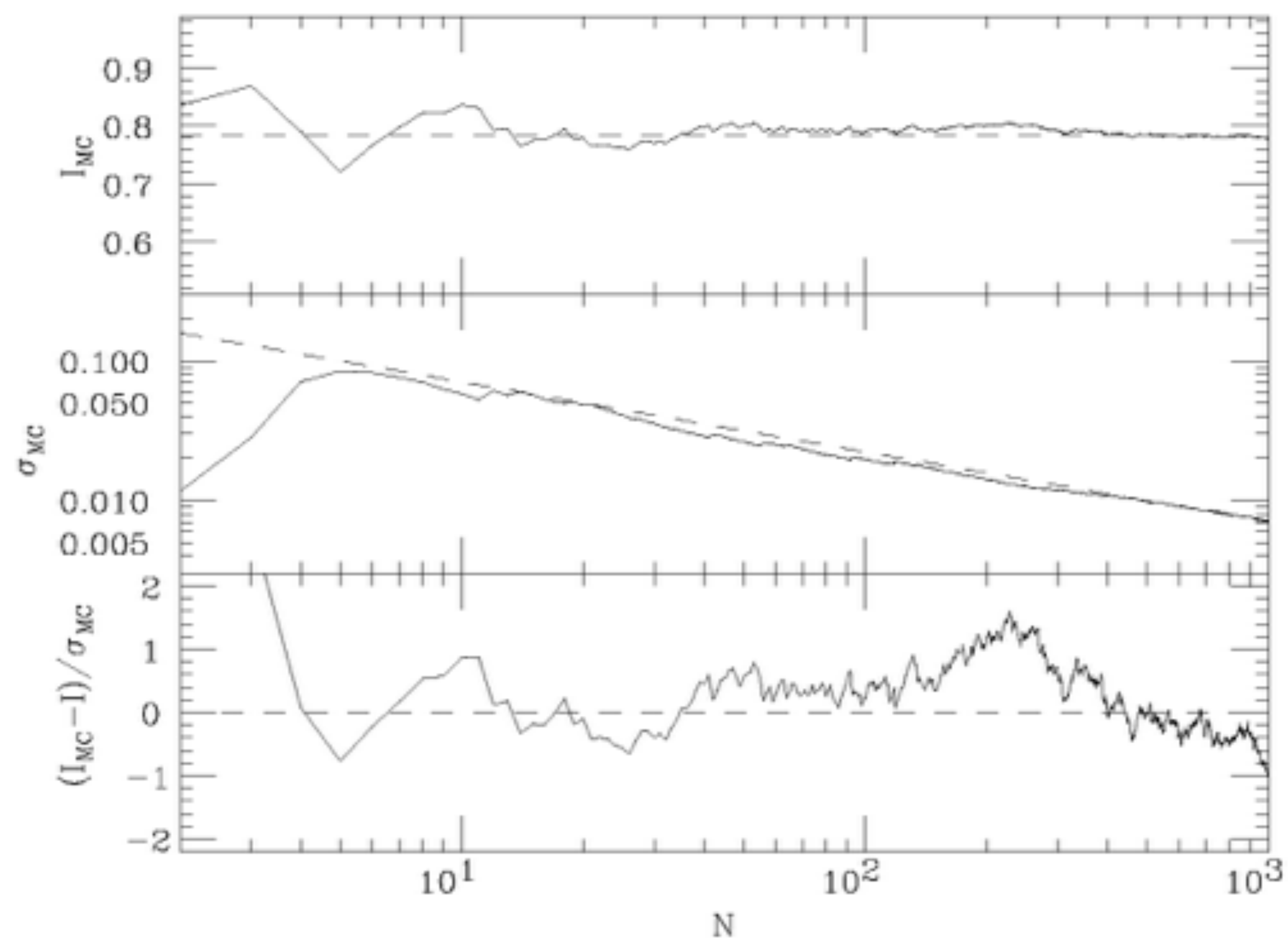
Convergence

- Monte Carlo integrals governed by Central Limit Theorem: error $\propto 1/\sqrt{N}$

c.f. trapezium rule $\propto 1/N^2$

Simpson's rule $\propto 1/N^4$

only if derivatives exist and are finite, e.g. $\sqrt{1-x^2} \sim 1/N^{3/2}$



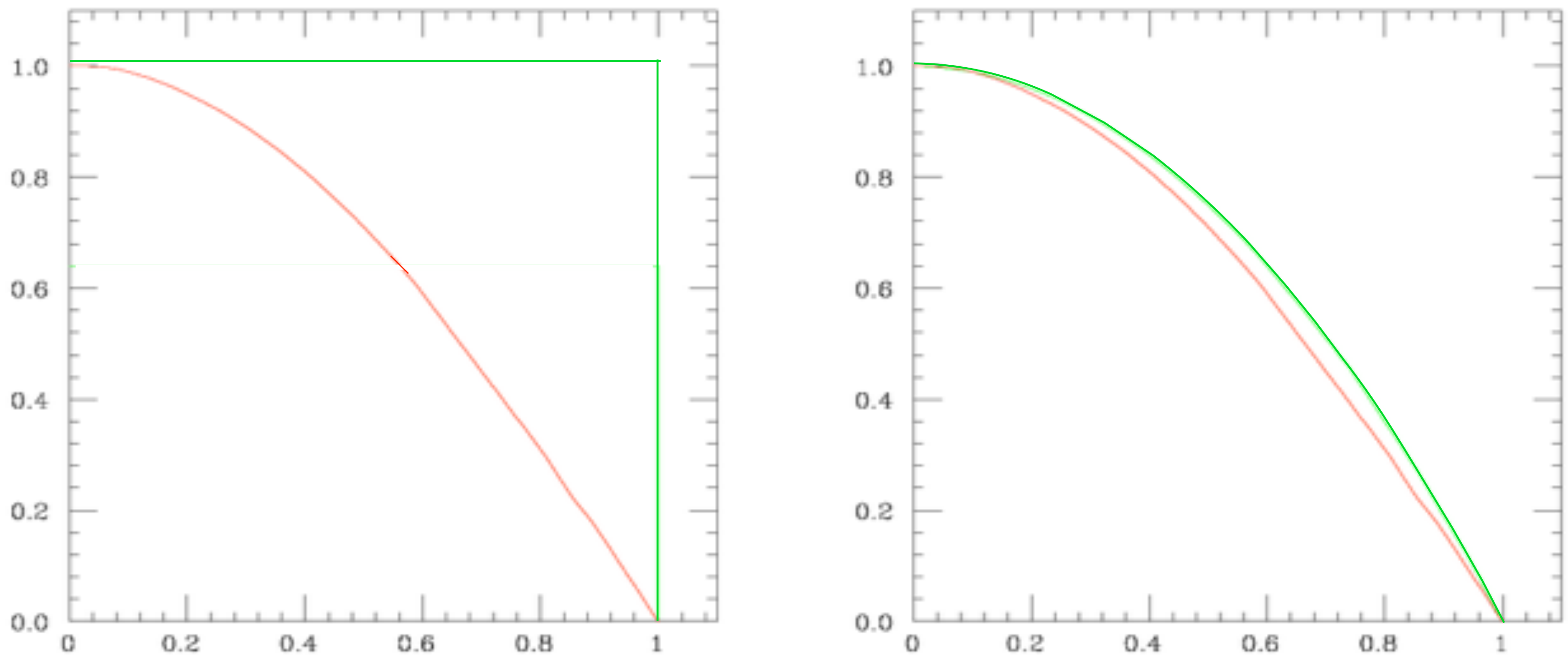
$$I = \int_0^1 \sqrt{1-x^2}\,dx = \frac{\pi}{4} = 0.785$$

$$\sqrt{V} = \sqrt{\frac{2}{3} - \frac{\pi^2}{16}} = 0.223$$

$$I = 0.785 \pm \frac{0.223}{\sqrt{N}}$$

Importance Sampling

- Convergence is improved by putting more points in regions where integrand is largest
- Corresponds to a Jacobian transformation
- Variance is reduced (weights "flattened")



$$
\begin{aligned}
I &= \int_0^1 dx \cos\tfrac{\pi}{2}x \\
&= 0.637 \pm 0.308/\sqrt{N}
\end{aligned}
$$

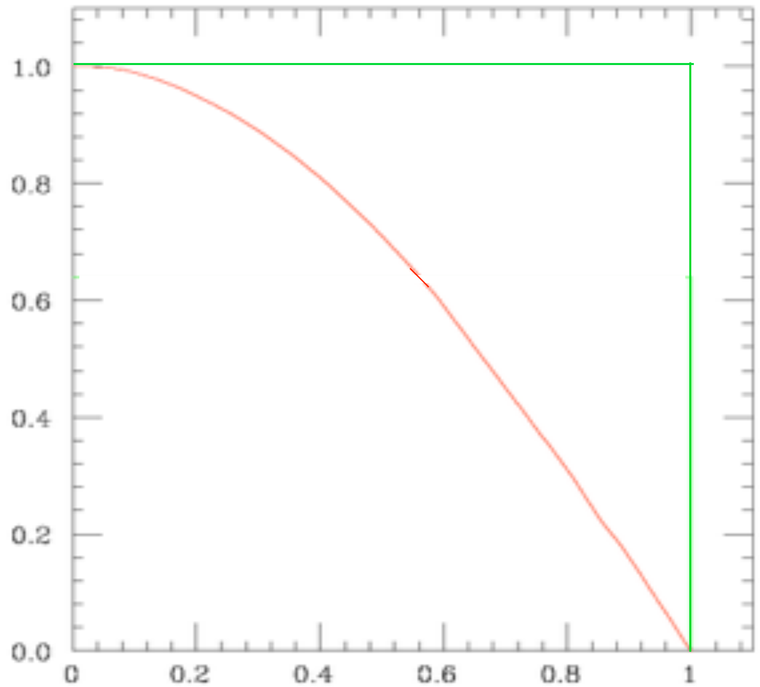
$$\frac{2}{\pi} \qquad \sqrt{\frac{1}{2}-\frac{4}{\pi^2}}$$

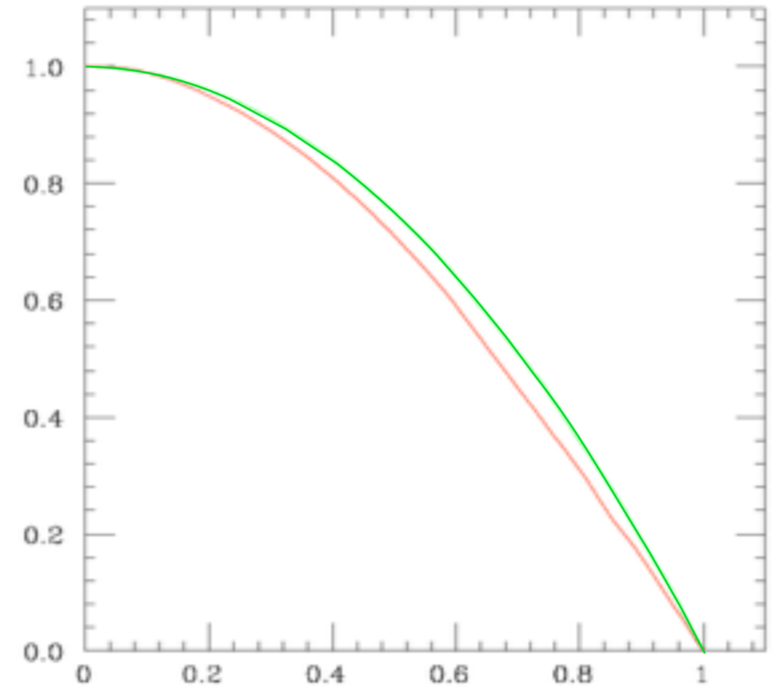
$$
\begin{aligned}
I &= \int_0^1 dx(1-x^2)\,\frac{\cos\frac{\pi}{2}x}{1-x^2} \\
&= \int_0^{2/3} d\rho\,\frac{\cos\frac{\pi}{2}x}{1-x^2}[x(\rho)] \\
&= 0.637 \pm 0.032/\sqrt{N}
\end{aligned}
$$

$$\rho = x - \frac{x^3}{3}$$

Hit-and-Miss

- Accept points with probability = w_i/w_{max} (provided all $w_i \geq 0$)
- Accepted points are distributed like real events
- MC efficiency $\varepsilon_{MC} = E[w]/w_{max}$ improved by importance sampling





$$\varepsilon_{\mathrm{MC}} = 1/I = 2/\pi = 64\%$$

$$\sigma = \sqrt{\frac{\varepsilon_{\mathrm{MC}}(1-\varepsilon_{\mathrm{MC}})}{N}} = \frac{0.48}{\sqrt{N}}$$

$$\varepsilon_{\mathrm{MC}} = \int_0^1 dx(1-x^2)/I = 3/\pi = 95\%$$

$$\sigma = \sqrt{\frac{\varepsilon_{\mathrm{MC}}(1-\varepsilon_{\mathrm{MC}})}{N}} = \frac{0.21}{\sqrt{N}}$$

Multi-dimensional Integration

- Formalism extends trivially to many dimensions
- Particle physics: very many dimensions,

  e.g. phase space = 3 dimensions per particles,

  LHC event ~ 250 hadrons.
- Monte Carlo error remains $\propto 1/\sqrt{N}$
- Trapezium rule $\propto 1/N^{2/d}$
- Simpson's rule $\propto 1/N^{4/d}$

Monte Carlo: Summary

Disadvantages of Monte Carlo:

- Slow convergence in few dimensions.

Advantages of Monte Carlo:

- Fast convergence in many dimensions.
- Arbitrarily complex integration regions (finite discontinuities not a problem).
- Few points needed to get first estimate ("feasibility limit").
- Every additional point improves accuracy ("growth rate").
- Easy error estimate.
- Hit-and-miss allows unweighted event generation, i.e. points distributed in phase space just like real events.

Phase Space Generation

$$\sigma = \frac{1}{2s}\int |\mathcal{M}|^2 \, d\Pi_n(\sqrt{s})$$
$$\Gamma = \frac{1}{2M}\int |\mathcal{M}|^2 \, d\Pi_n(M)$$

- Phase space:

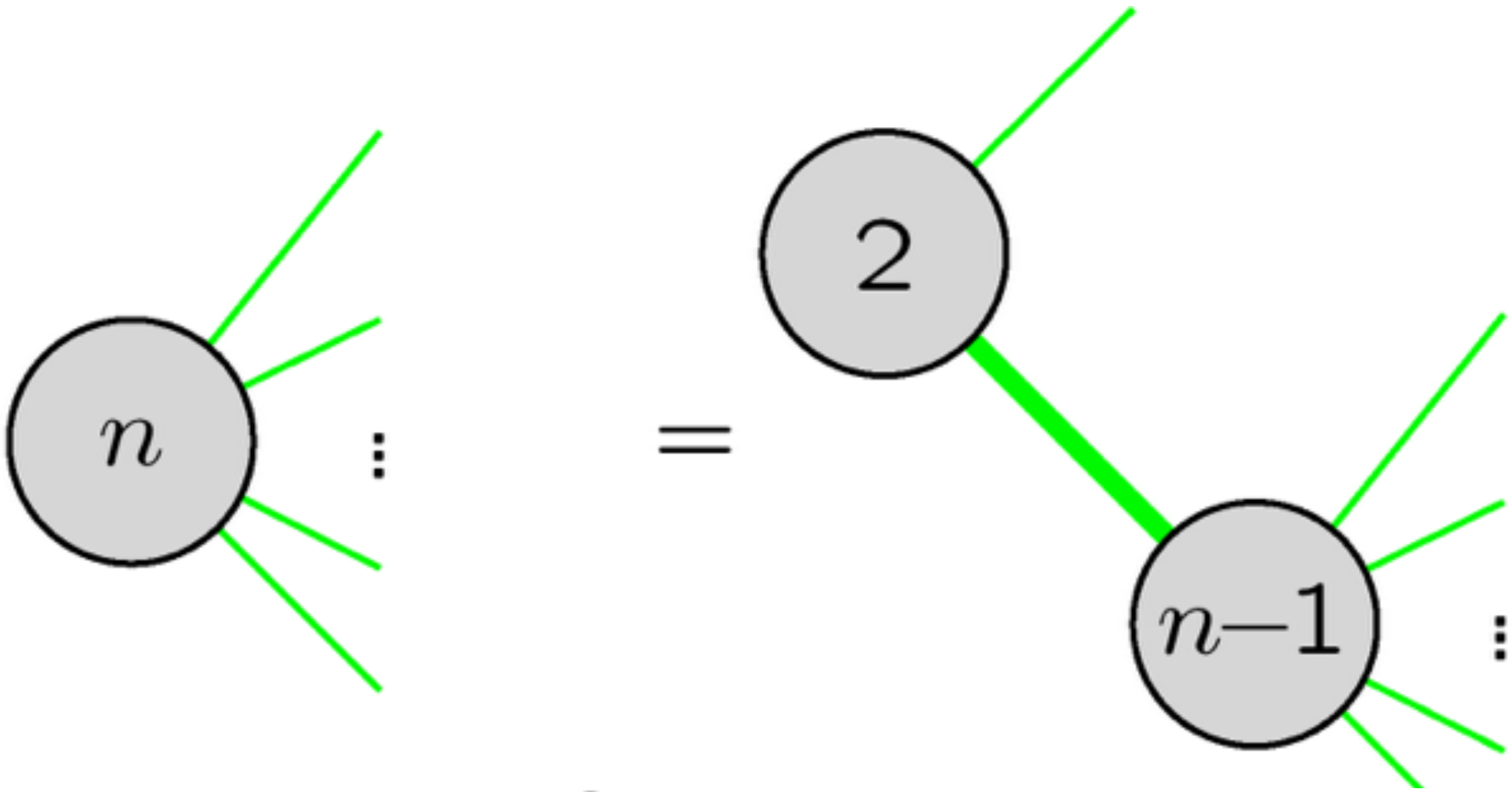
$$d\Pi_n(M) = \left[\prod_{i=1}^{n} \frac{d^3p_i}{(2\pi)^3(2E_i)}\right](2\pi)^4\delta^{(4)}\left(p_0 - \sum_{i=1}^{n} p_i\right)$$

- Two-body easy:

$$d\Pi_2(M) = \frac{1}{8\pi}\,\frac{2p}{M}\,\frac{d\Omega}{4\pi}$$

Phase Space Generation

- Other cases by recursive subdivision:



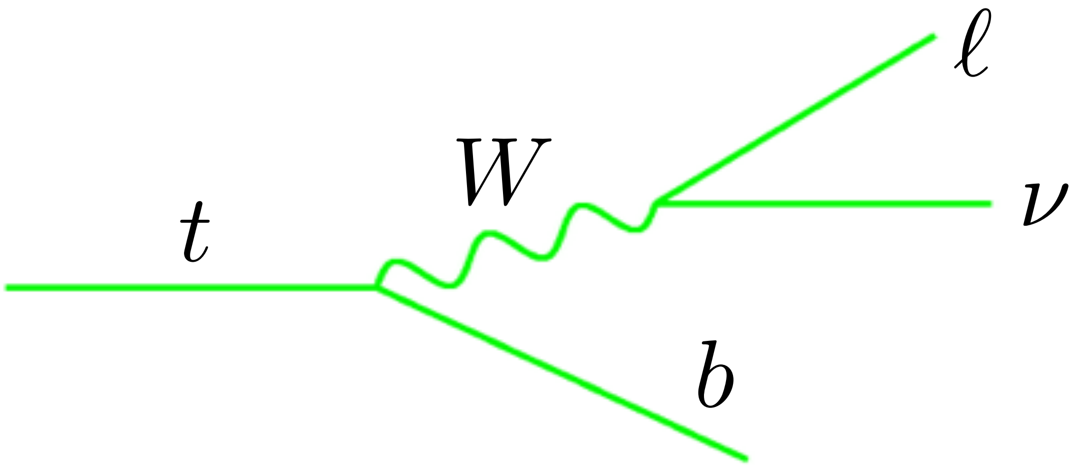
$$d\Pi_n(M) = \frac{1}{2\pi}\int_0^{(M-m)^2} dm_x^2 \, d\Pi_2(M)\, d\Pi_{n-1}(m_x)$$

- Or by 'democratic' algorithms: RAMBO, MAMBO
  Can be better, but matrix elements rarely flat.

Particle Decays

- Simplest example

  e.g. top quark decay:



$$|\mathcal{M}|^2 = \frac{1}{2}\left(\frac{8\pi\alpha}{\sin^2\theta_w}\right)^2 \frac{p_t\cdot p_\ell\, p_b\cdot p_\nu}{(m_W^2 - M_W^2)^2 + \Gamma_W^2 M_W^2}$$

$$\Gamma = \frac{1}{2M}\frac{1}{128\pi^3}\int |\mathcal{M}|^2 dm_W^2 \left(1 - \frac{m_W^2}{M^2}\right)\frac{d\Omega}{4\pi}\frac{d\Omega_W}{4\pi}$$

Breit-Wigner peak of W very strong - but can be removed by importance sampling:

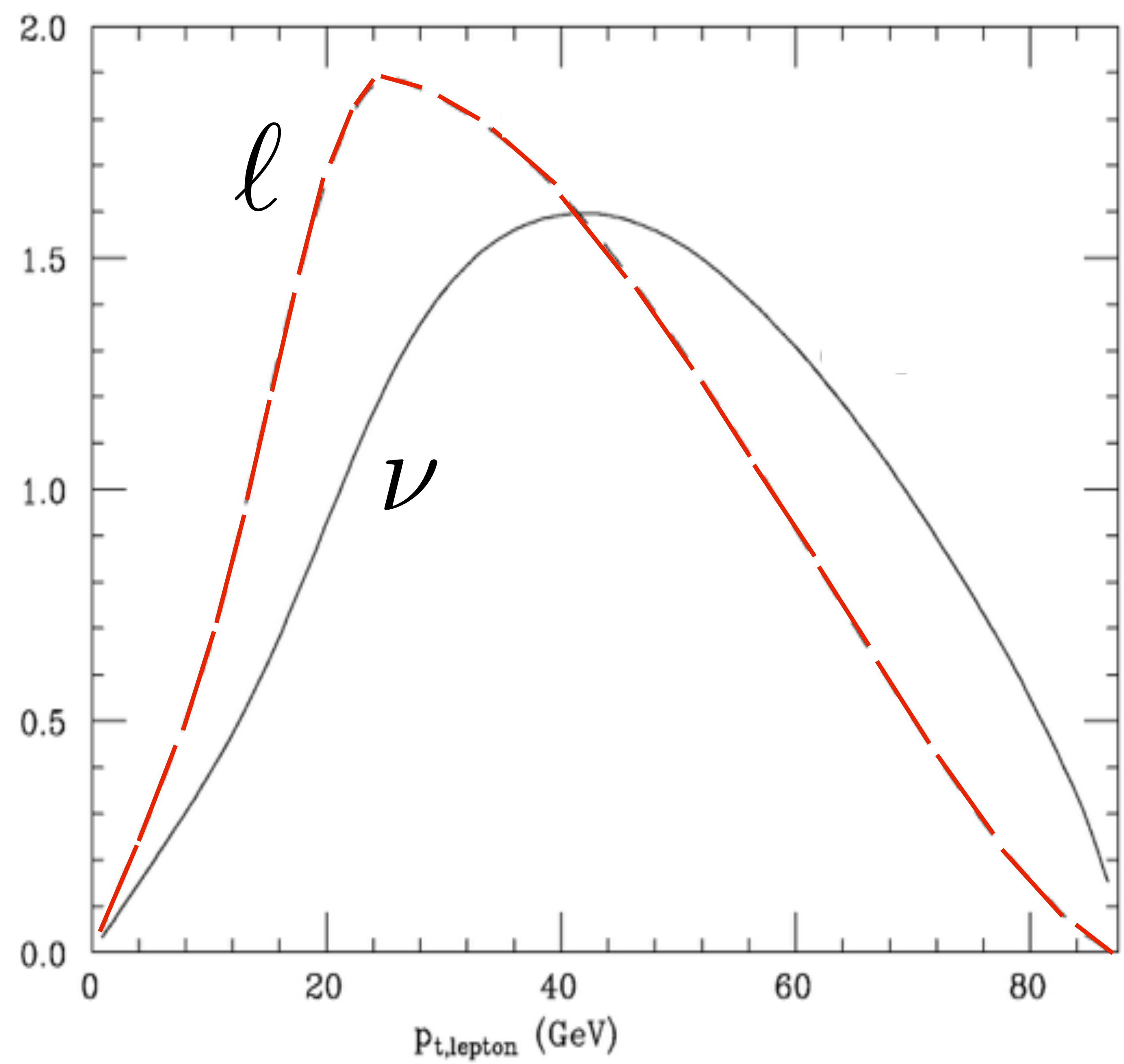
$$m_W^2 \to \arctan\left(\frac{m_W^2 - M_W^2}{\Gamma_W M_W}\right)$$ (prove it!)

Associated Distributions

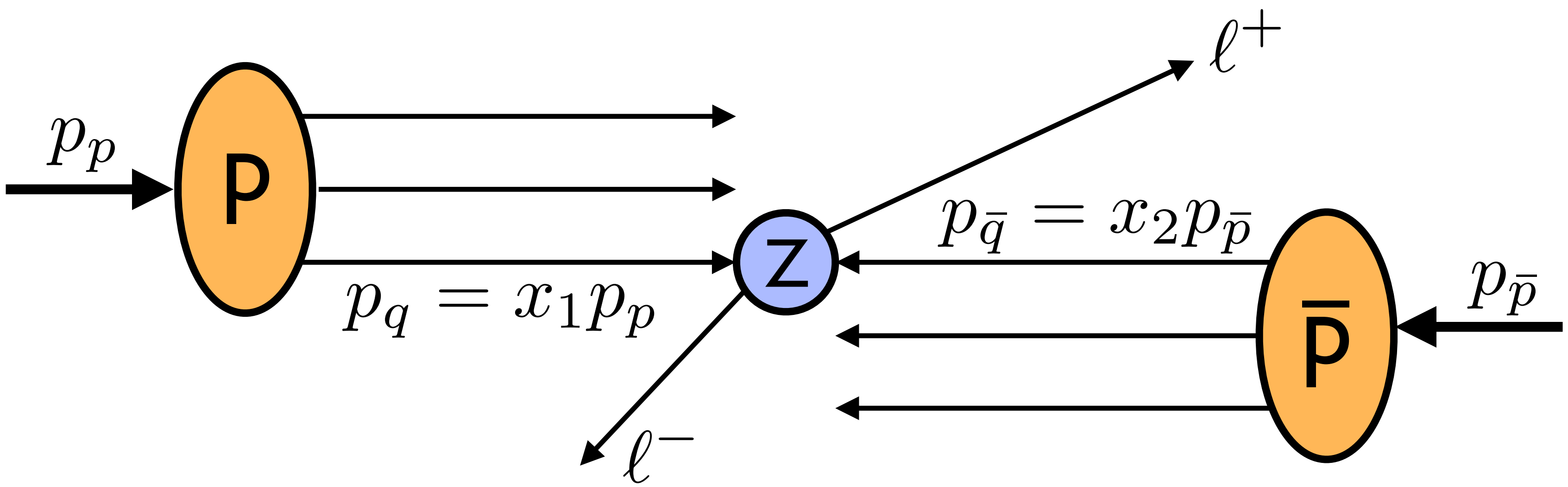
Big advantage of Monte Carlo integration:

- Simply histogram any associated quantities.
- Almost any other technique requires new integration for each observable.
- Can apply arbitrary cuts/ smearing.

e.g. lepton momentum in top decays:



Hadron-Hadron Cross Sections



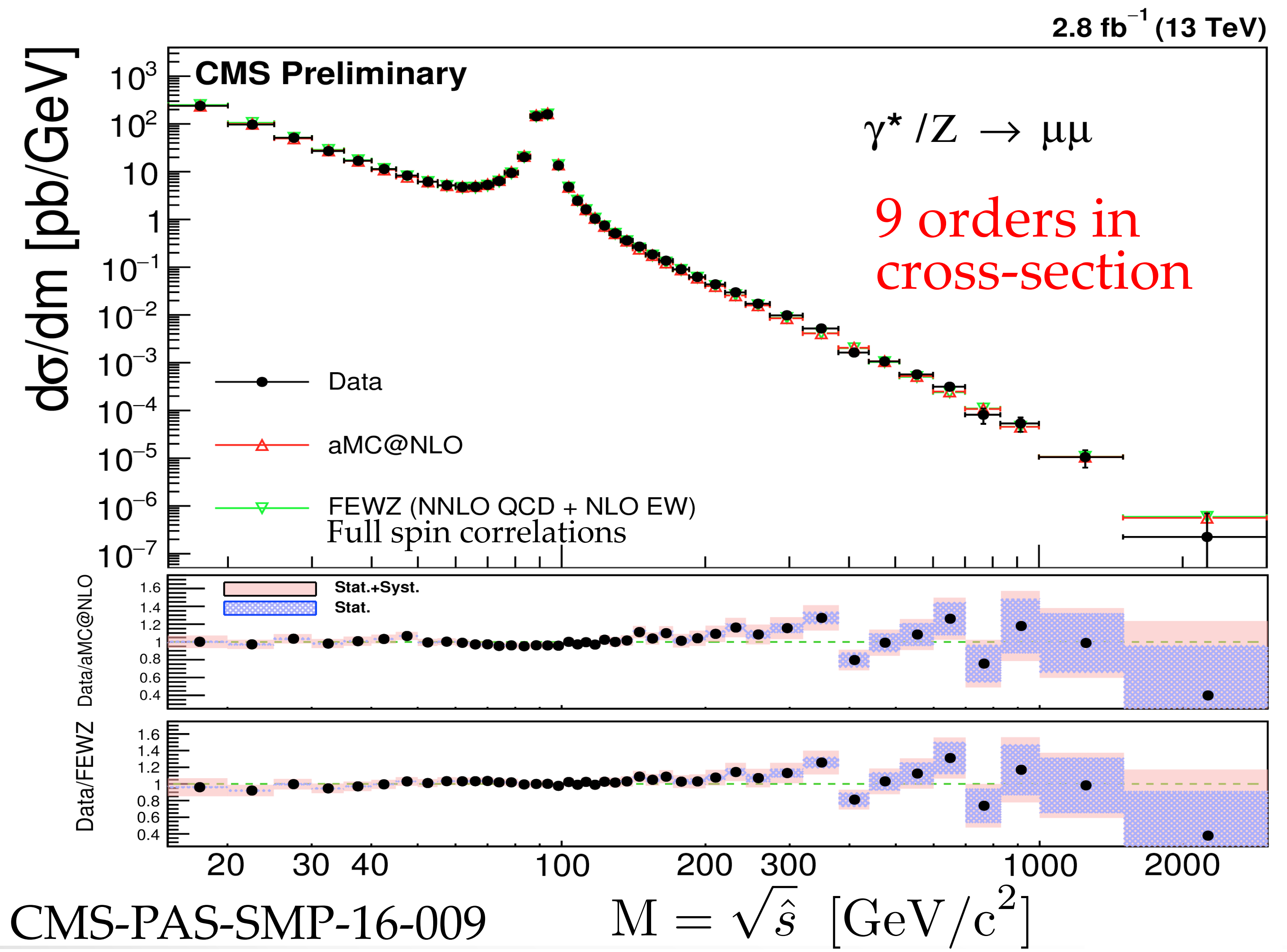
$$s = E_{\rm cm}^2 = 4p_p p_{\bar p} \qquad \hat{s} = 4p_q p_{\bar q} = x_1 x_2 s$$

- Consider e.g. $p\bar{p} \to Z^0 \to \ell^+\ell^-$
- Integrations over incoming parton momentum distributions:

$$\sigma(s) = \int_0^1 dx_1 f(x_1) \int_0^1 dx_2 f(x_2)\, \hat\sigma(x_1 x_2 s)$$

- Hard process cross section $\hat\sigma(\hat s)$ has strong peak, due to Z^0 resonance: needs importance sampling (like W in top decay)

$pp \to \ell^+\ell^-$ cross section



$$\hat{\sigma}_{q\bar{q}\to Z^0\to\ell^+\ell^-} = \frac{4\pi\hat{s}}{3M_Z^2}\frac{\Gamma_\ell\Gamma_q}{(\hat{s}-M_Z^2)^2+\Gamma_Z^2M_Z^2}$$

- "Background" is $q\bar{q}\to\gamma^*\to\ell^+\ell^-$

Parton-Level Monte Carlo Calculations

Now we have everything we need to make parton-level cross section calculations and distributions

Can be largely automated…

- MADGRAPH
- GRACE
- COMPHEP
- AMEGIC++
- ALPGEN

But…

- Fixed parton/jet multiplicity
- No control of large higher-order corrections
- Parton level

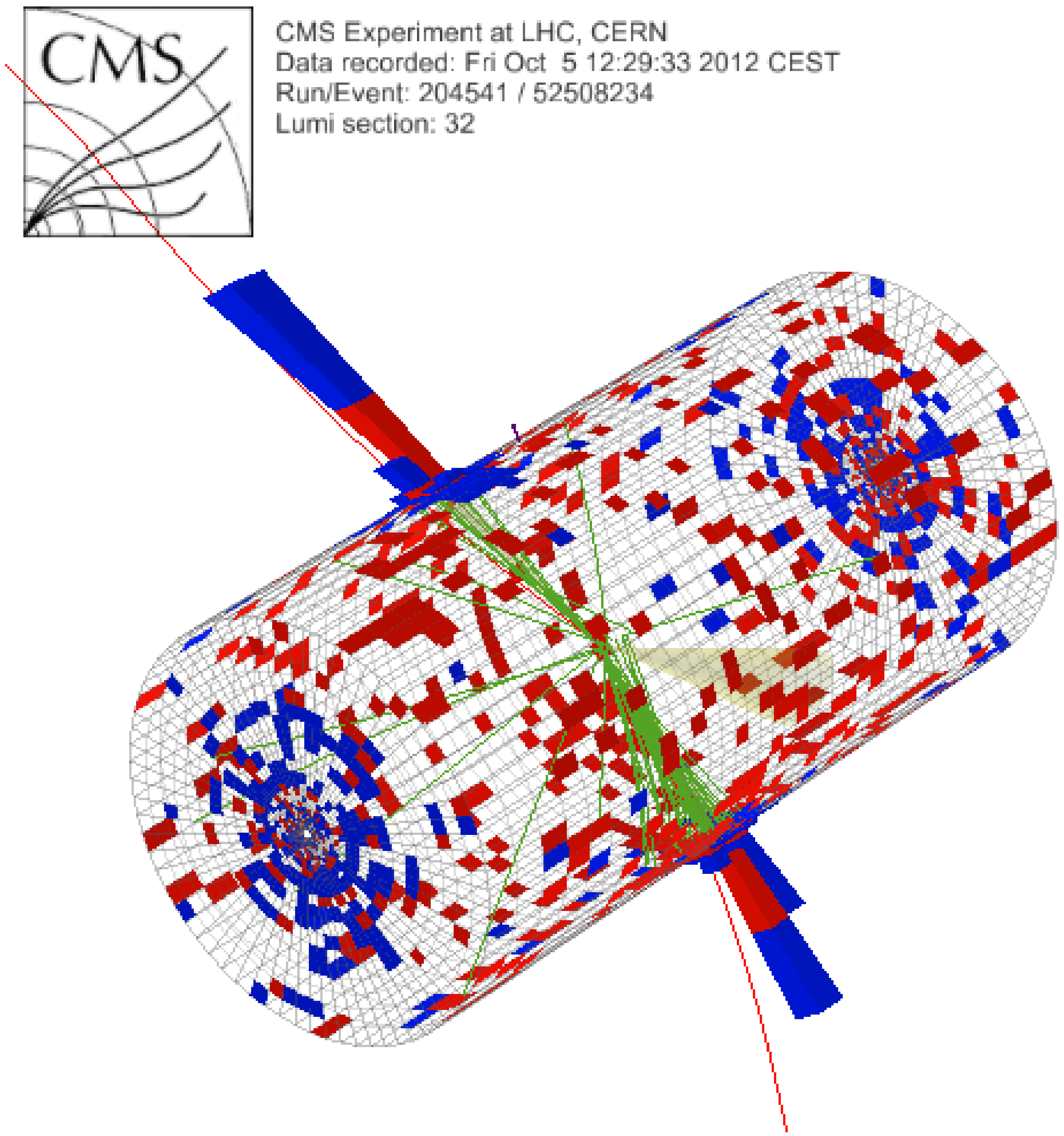
→ Need hadron level event generators

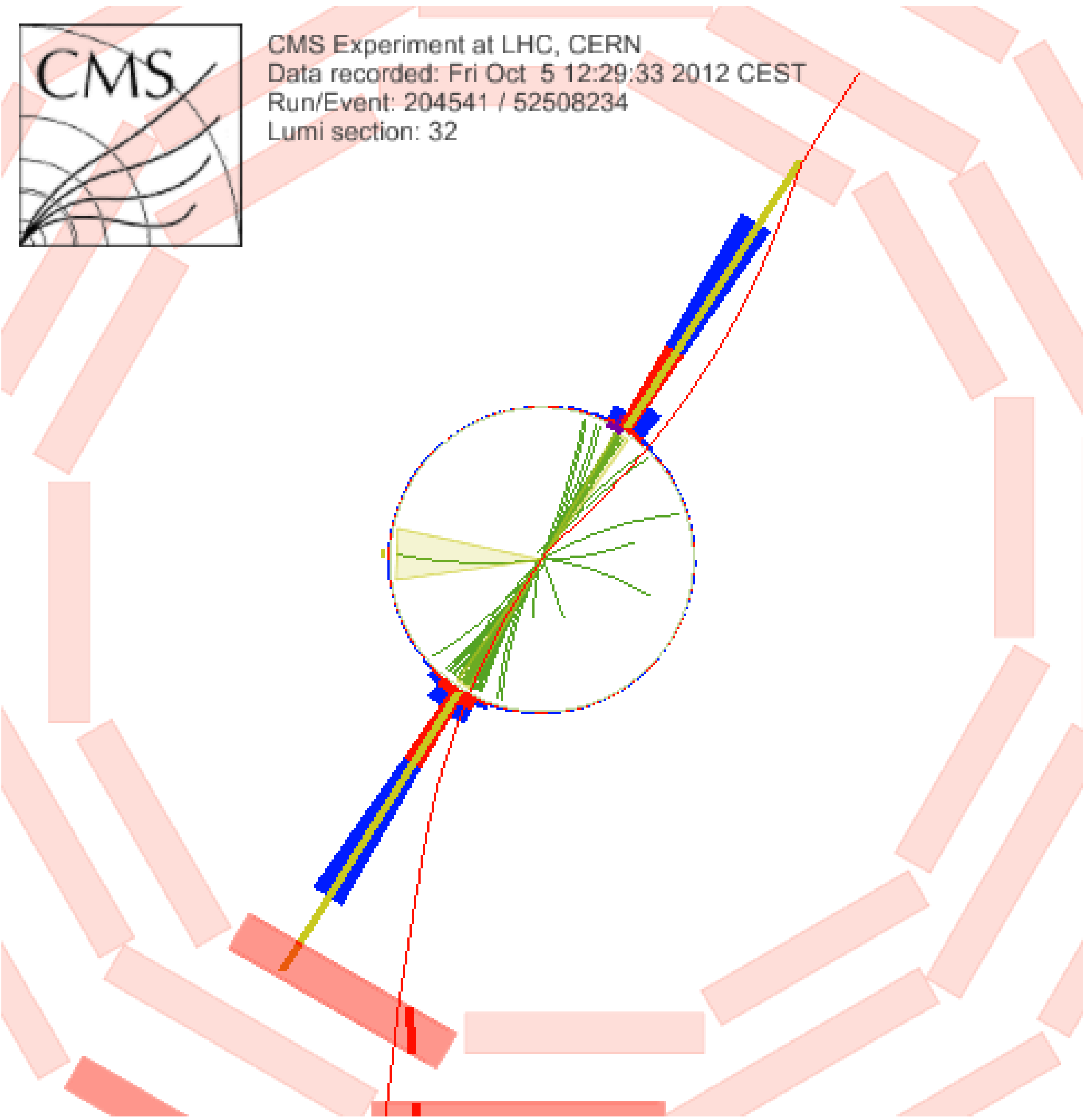
Monte Carlo Event Generation

Monte Carlo Event Generation

- Monte Carlo event generation:
  - theoretical status and limitations
- Recent improvements:
  - perturbative and non-perturbative
- Overview of results:
  - W, Z, top, Higgs, BSM (+jets)

A high-mass dijet event

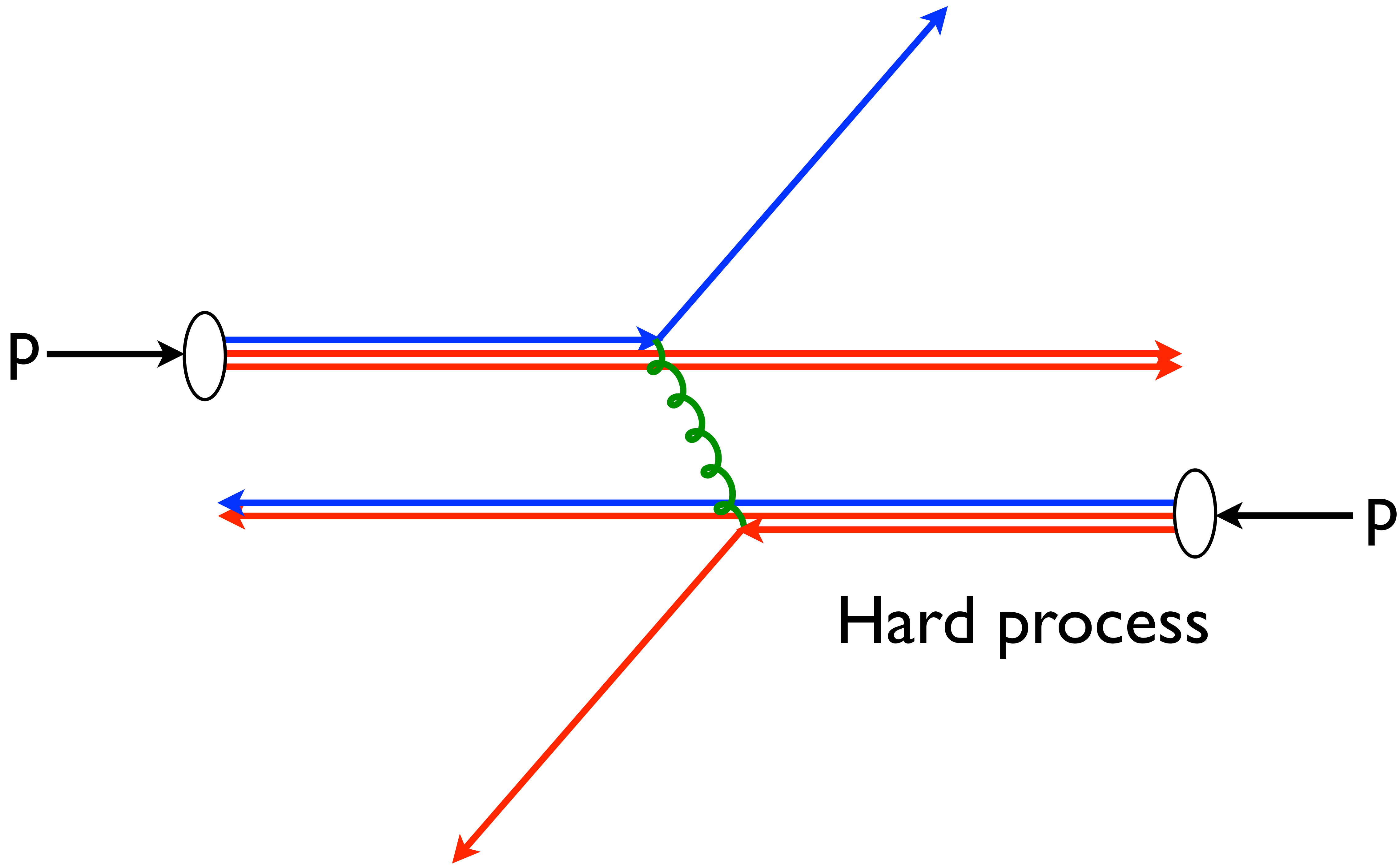




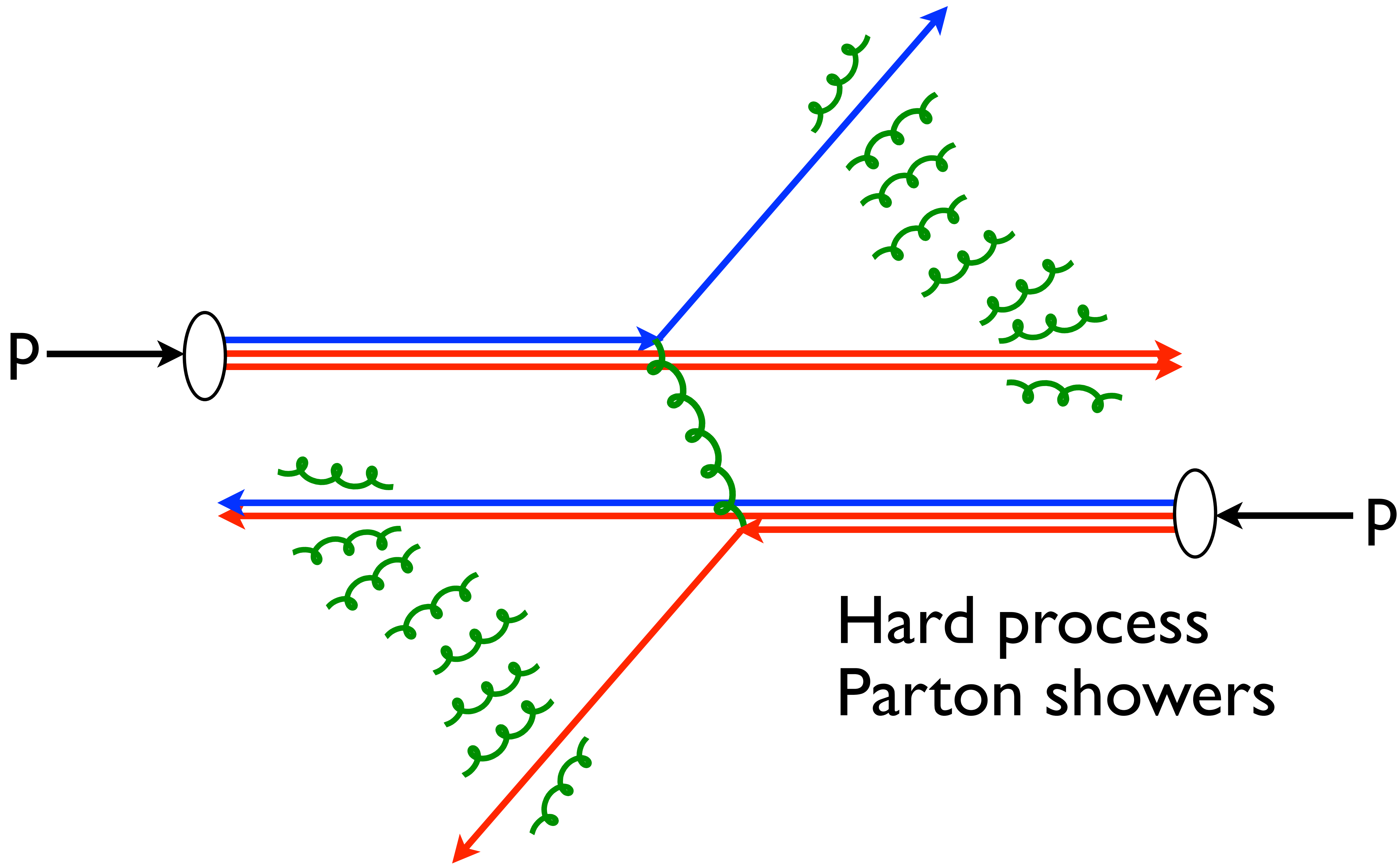
- M_{jj} = 5.15 TeV

CMS PAS EXO-12-059

LHC dijet

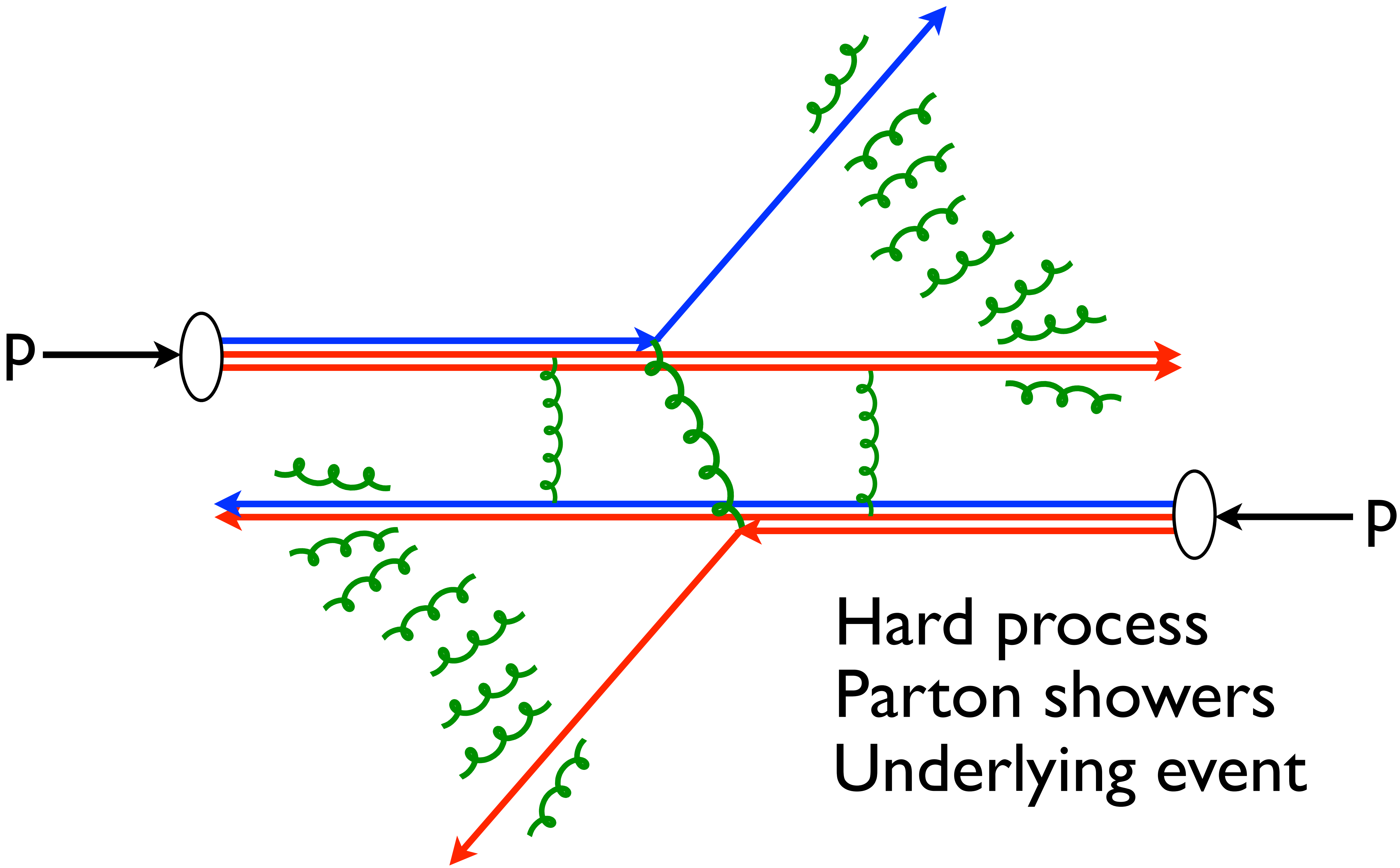


LHC dijet



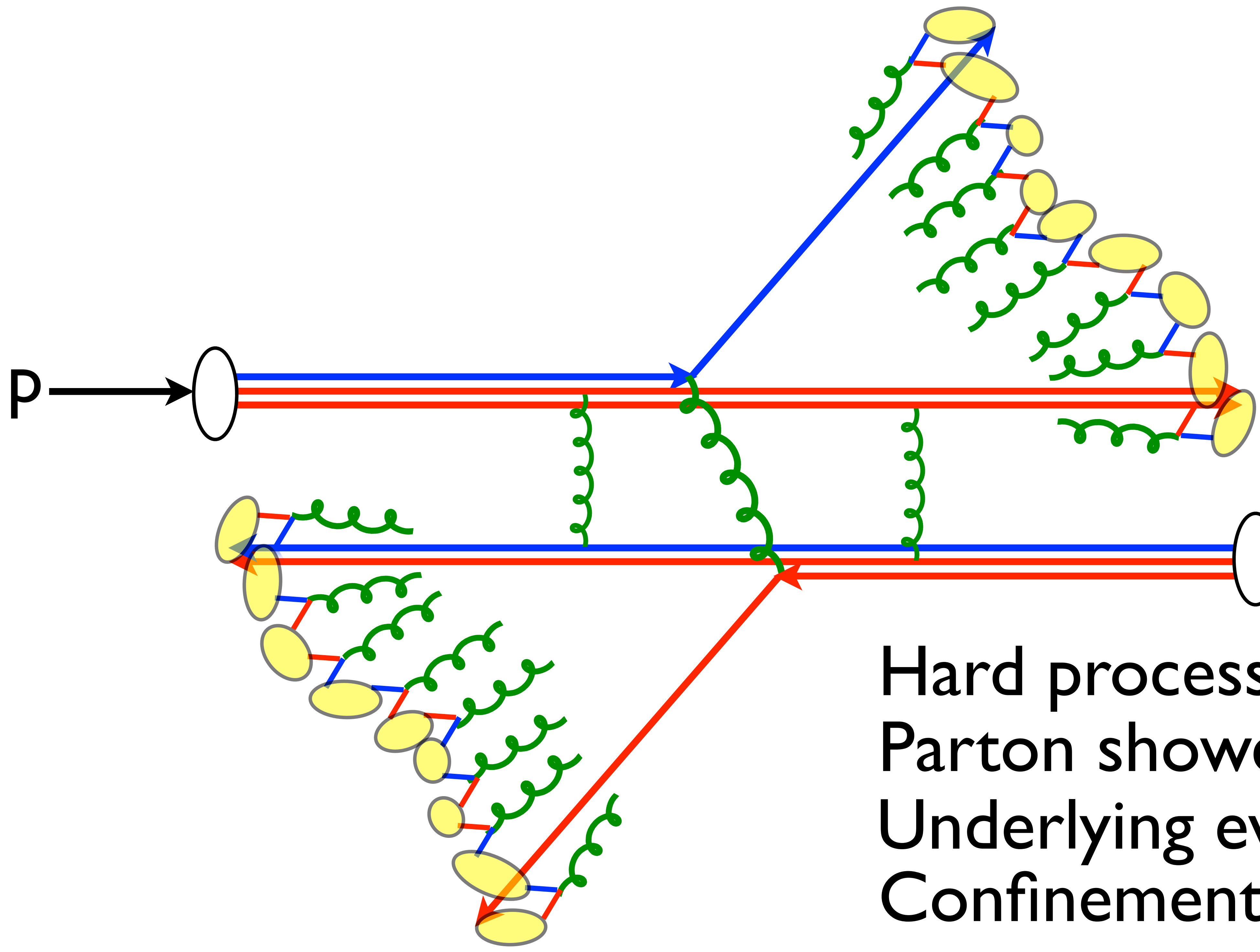
Hard process
Parton showers

LHC dijet



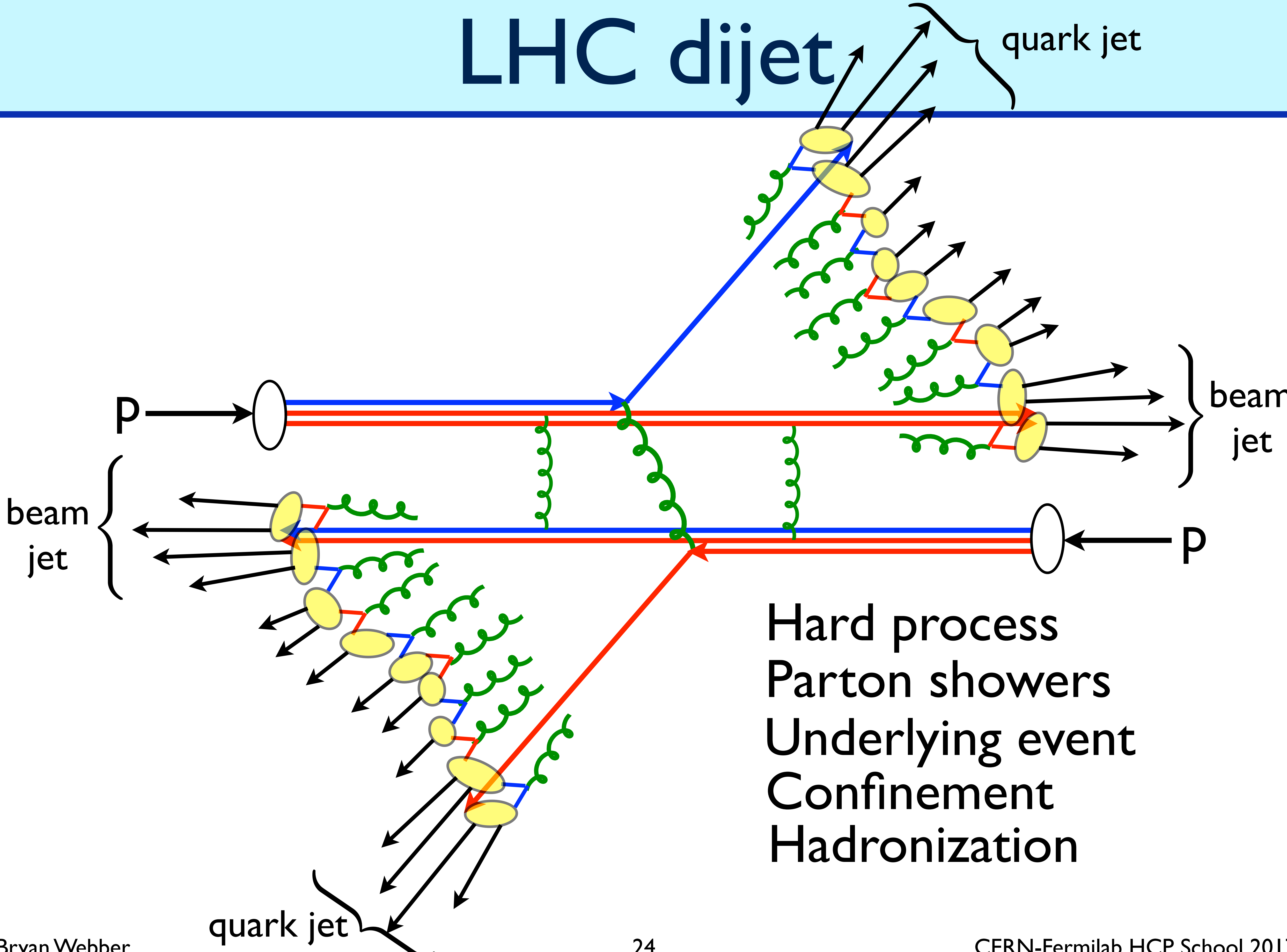
Hard process
Parton showers
Underlying event

LHC dijet



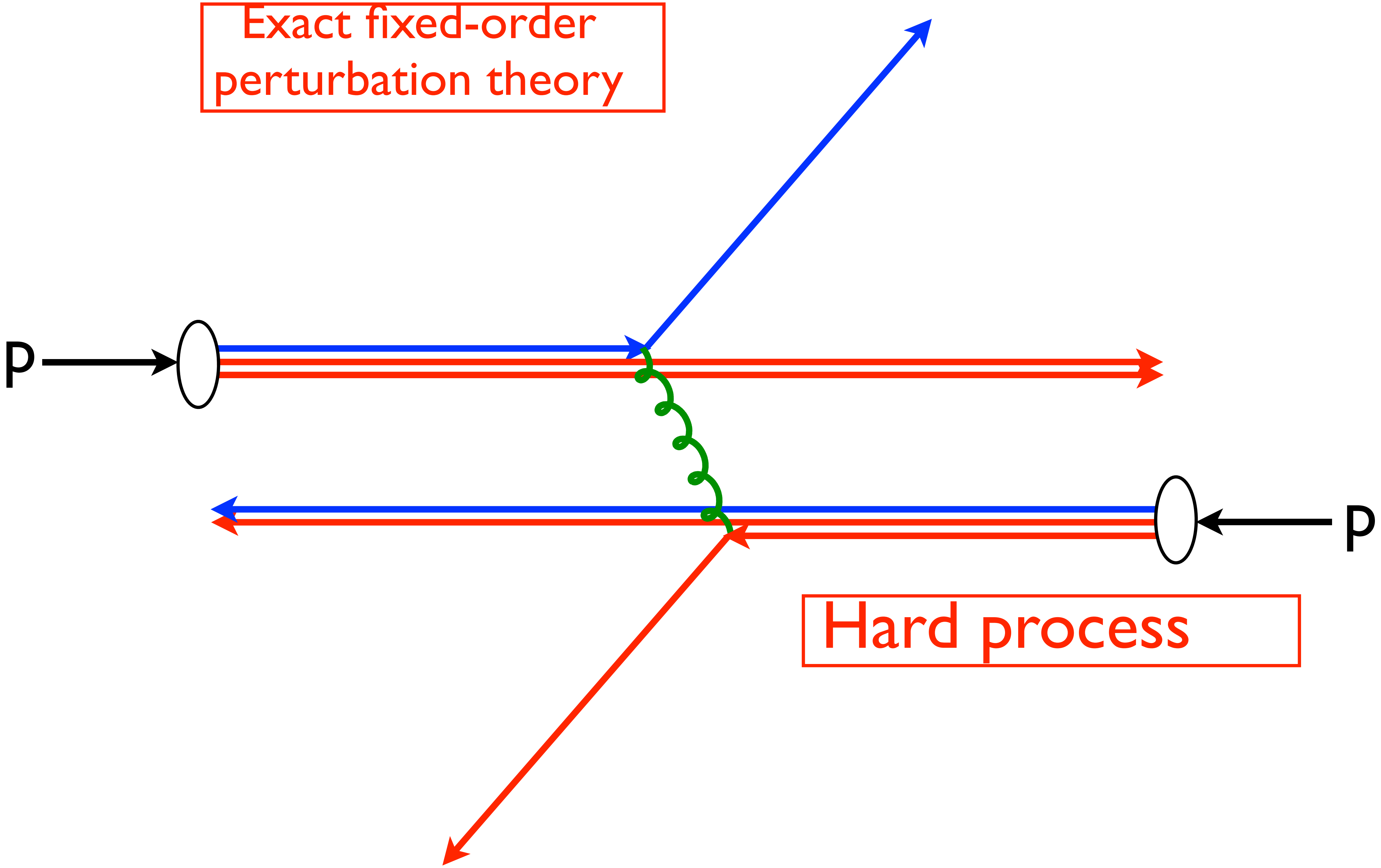
Hard process
Parton showers
Underlying event
Confinement

LHC dijet

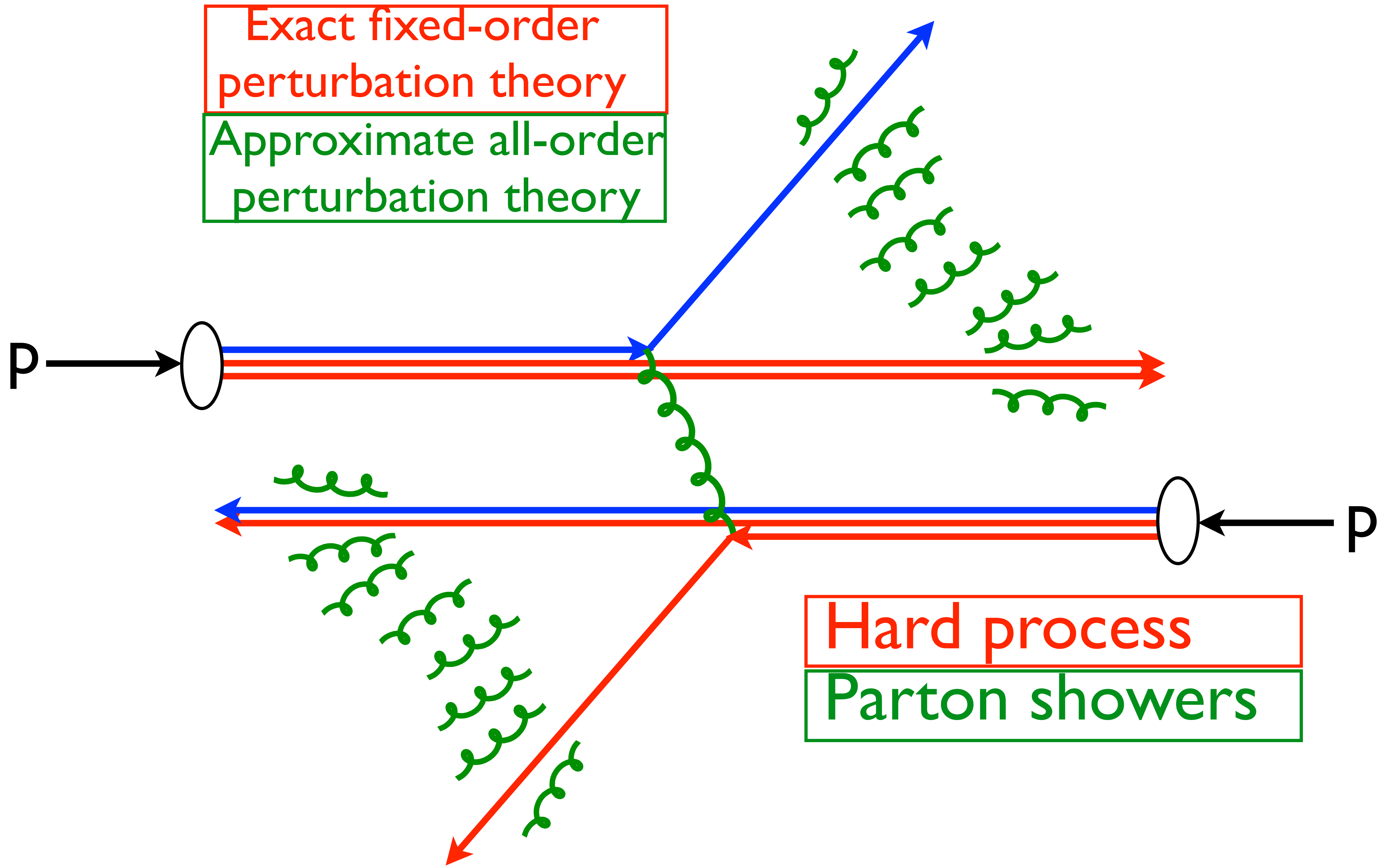


Hard process
Parton showers
Underlying event
Confinement
Hadronization

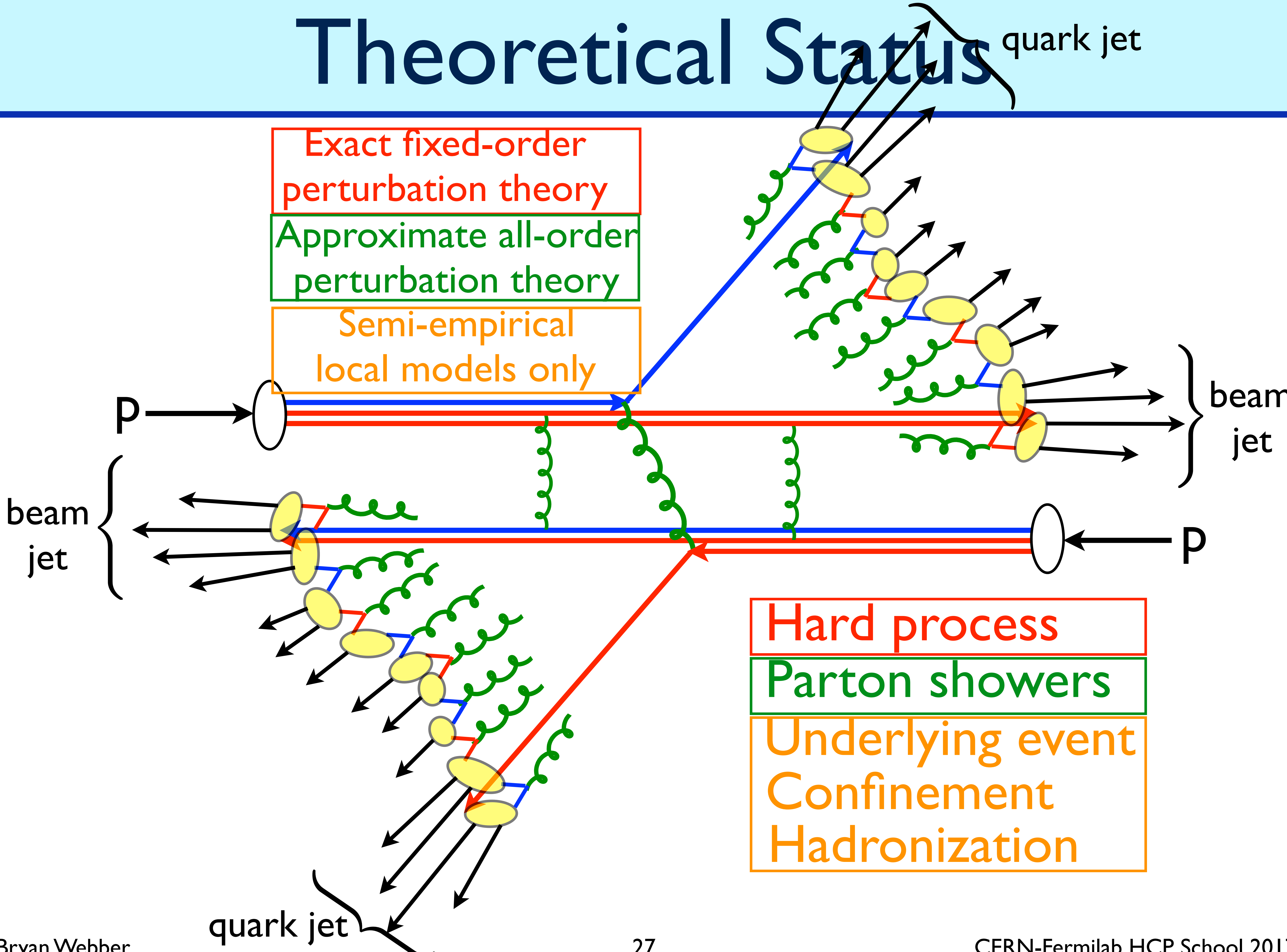
Theoretical Status



Theoretical Status



Theoretical Status



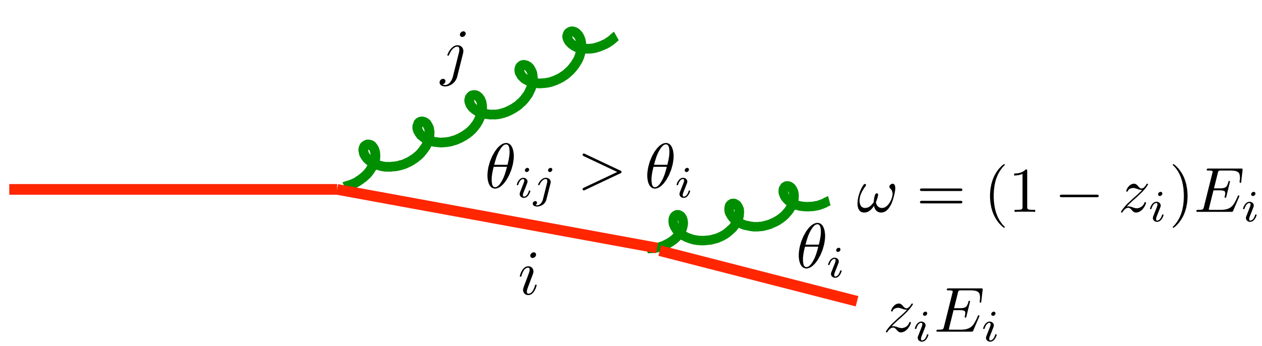
QCD Factorization

$$\sigma_{pp\to X}(E_{pp}^2) = \int_0^1 \underset{\text{momentum fractions}}{dx_1\,dx_2}\; \underbrace{f_i(x_1,\mu^2)\,f_j(x_2,\mu^2)}_{\text{parton distributions at scale }\mu^2}\; \underbrace{\hat\sigma_{ij\to X}(x_1x_2E_{pp}^2,\mu^2)}_{\text{hard process cross section}}$$

- Jet formation and underlying event take place over a much longer time scale, with unit probability
- Hence they cannot affect the cross section
- Scale dependences of parton distributions and hard process cross section are perturbatively calculable, and cancel order by order

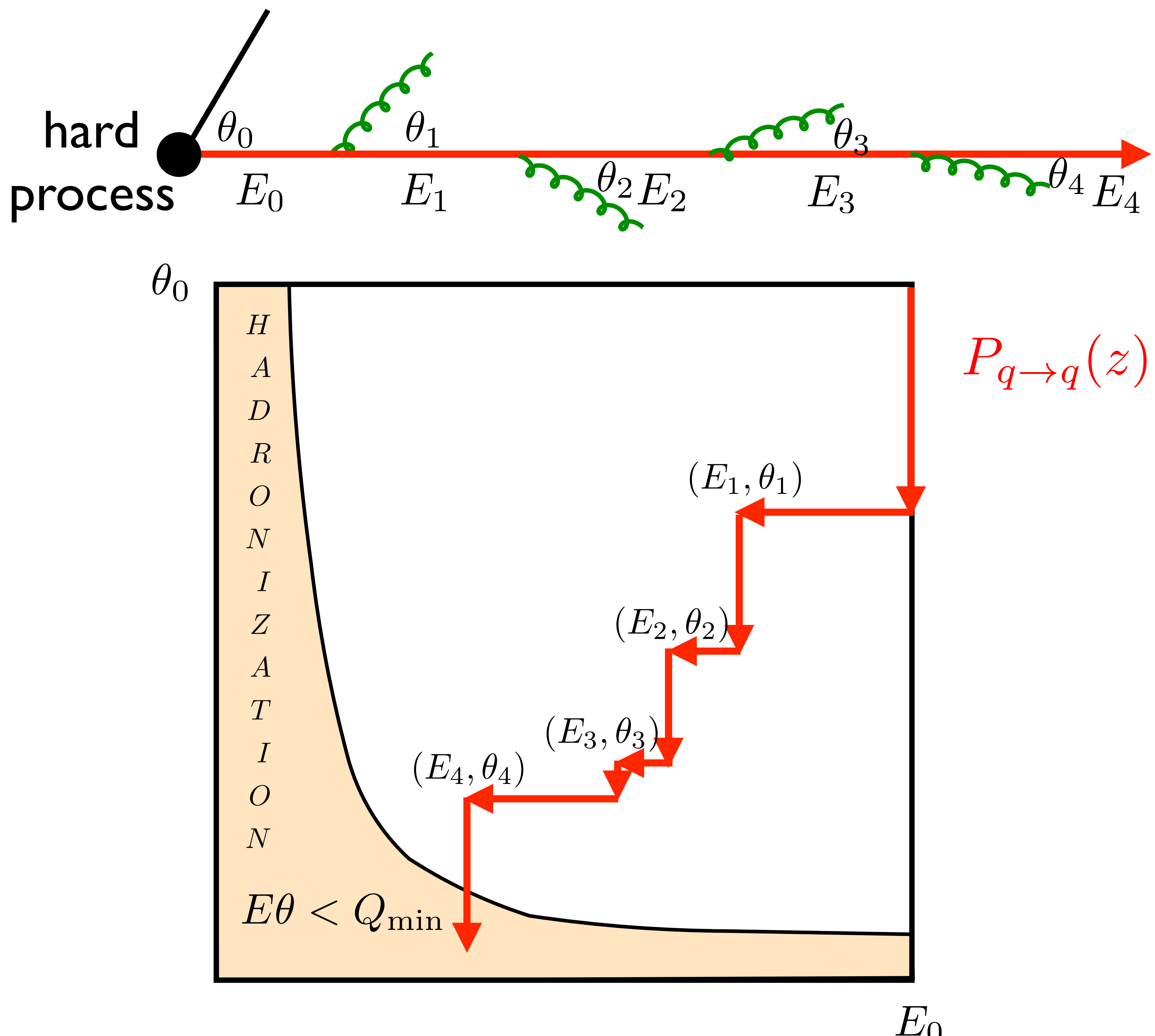
Parton Shower Approximation

- Keep only most singular parts of QCD matrix elements:
- Collinear $$d\sigma_{n+1} \approx \frac{\alpha_S}{2\pi}\sum_i P_{ii}(z_i,\phi_i)\,dz_i\,\frac{d\xi_i}{\xi_i}\frac{d\phi_i}{2\pi}d\sigma_n \qquad \xi_i = 1-\cos\theta_i$$
- Soft $$\begin{aligned} d\sigma_{n+1} &\approx \frac{\alpha_S}{2\pi}\sum_{i,j}(-\mathbf{T}_i\cdot\mathbf{T}_j)\frac{p_i\cdot p_j}{p_i\cdot k\,p_j\cdot k}\omega\,d\omega\,d\xi_i\,\frac{d\phi_i}{2\pi}d\sigma_n \\ &= \frac{\alpha_S}{2\pi}\sum_{i,j}(-\mathbf{T}_i\cdot\mathbf{T}_j)\frac{\xi_{ij}}{\xi_i\,\xi_j}\frac{d\omega}{\omega}d\xi_i\,\frac{d\phi_i}{2\pi}d\sigma_n \\ &\approx \frac{\alpha_S}{2\pi}\sum_{i,j}(-\mathbf{T}_i\cdot\mathbf{T}_j)\,\Theta(\xi_{ij}-\xi_i)\frac{d\omega}{\omega}\frac{d\xi_i}{\xi_i}d\sigma_n \end{aligned}$$



→ Angular-ordered parton shower (or dipoles)

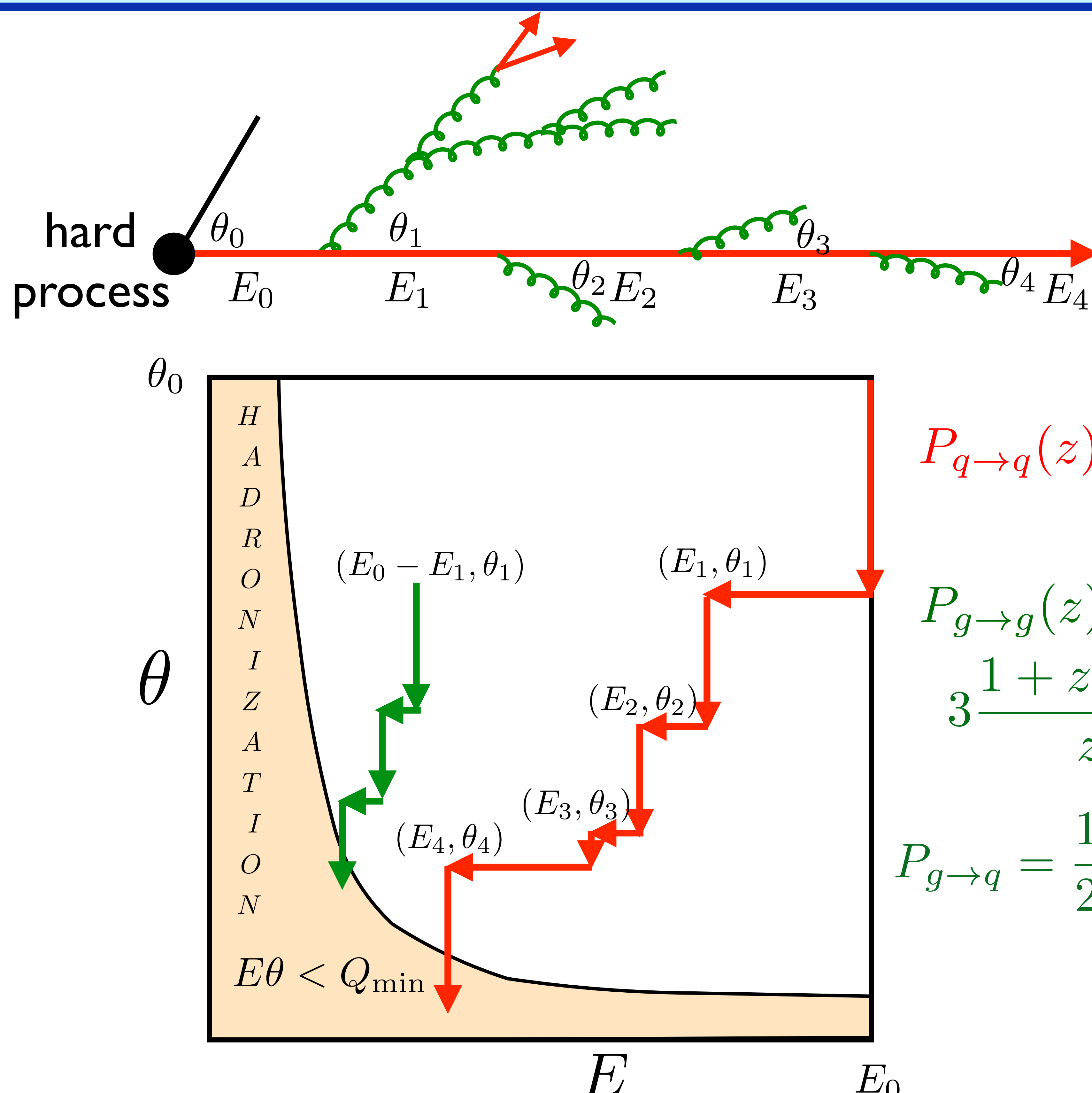
Parton Shower Evolution



$$z = \frac{E_{i+1}}{E_i}$$

$$P_{q\to q}(z) = \frac{4}{3}\frac{1+z^2}{1-z}$$

Parton Shower Evolution



$$z = \frac{E_{i+1}}{E_i}$$

$$P_{q\to q}(z) = \frac{4}{3}\frac{1+z^2}{1-z}$$

$$P_{g\to g}(z) = 3\frac{1+z^4+(1-z)^4}{z(1-z)}$$

$$P_{g\to q} = \frac{1}{2}\left[z^2+(1-z)^2\right]$$

Sudakov Factor

- $\Delta_i(Q,Q_{min})$ = probability for parton i to evolve from Q to Q_{min} without any resolvable emissions:

$$\begin{aligned}\Delta_i(Q_0,Q_{\rm min}) &\approx 1 - C_i\frac{\alpha_S}{\pi}\int^{E_0}\frac{d\omega}{\omega}\int^{\theta_0}2\frac{d\theta}{\theta}\Theta(\omega\theta-Q_{\rm min})+\ldots\\ &\approx 1 - C_i\frac{\alpha_S}{\pi}\ln^2\left(\frac{Q_0}{Q_{\rm min}}\right)+\ldots\\ &\approx \exp\left[-C_i\frac{\alpha_S}{\pi}\ln^2\left(\frac{Q_0}{Q_{\rm min}}\right)\right]\end{aligned}$$

- $C_q = C_F = 4/3$, $C_g = C_A = 3$

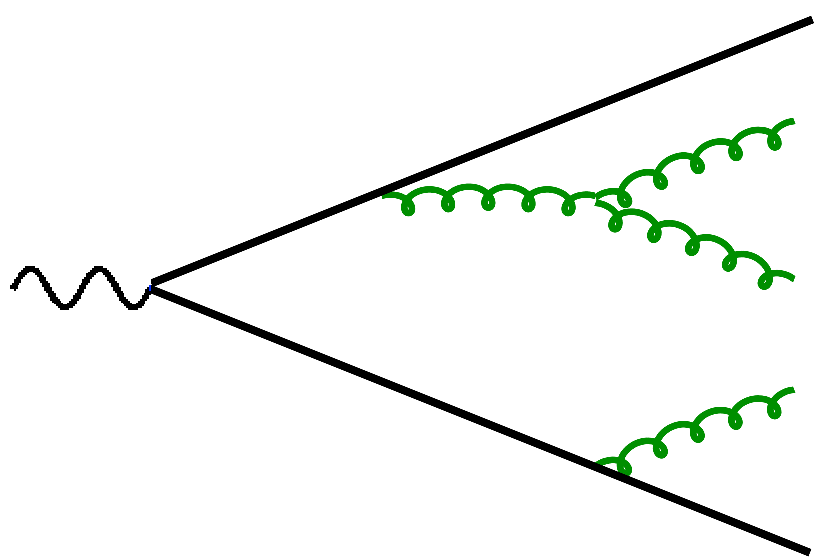
- Then probability to evolve from Q_1 to Q_2 without resolvable emissions is $\Delta_i(Q_1,Q_{min})/\Delta_i(Q_2,Q_{min})$

- Given Q_1, find Q_2 by solving

$$\boxed{\Delta_i(Q_1,Q_{min})/\Delta_i(Q_2,Q_{min}) = \text{Random \#}}$$

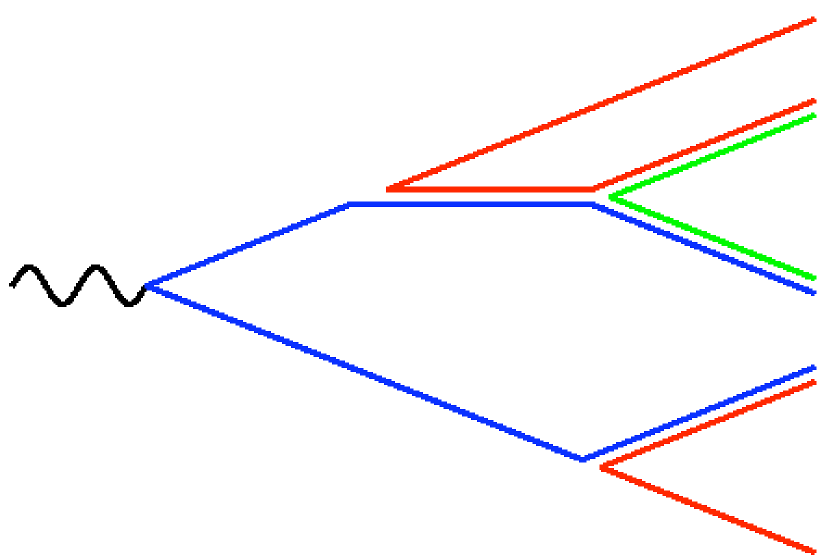
Hadronization Models

- In parton shower, relative transverse momenta evolve from a high scale Q towards lower values
- At a scale near Λ_{QCD}~200 MeV, perturbation theory breaks down and hadrons are formed
- Before that, at scales ~ few x Λ_{QCD}, there is universal preconfinement of colour
- Colour, flavour and momentum flows are only locally redistributed by hadronization



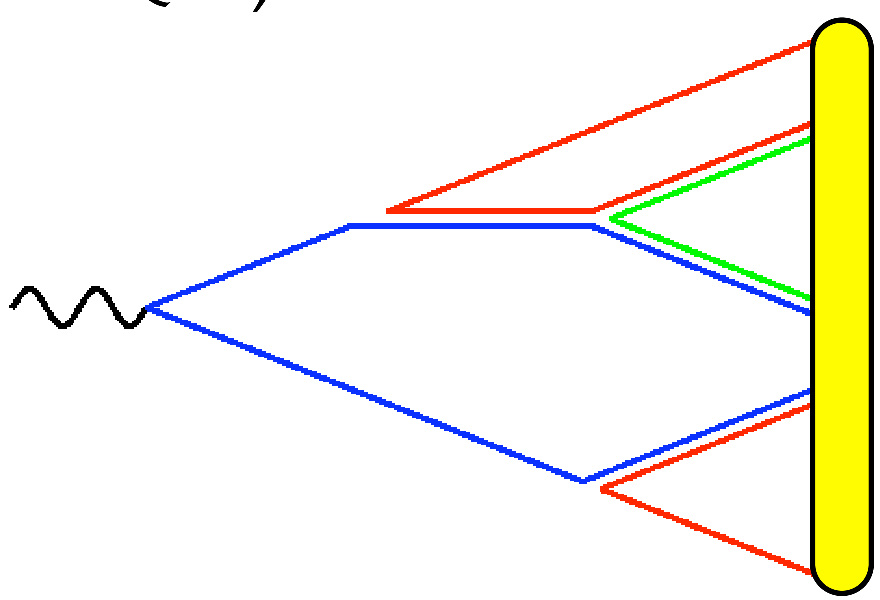
Hadronization Models

- In parton shower, relative transverse momenta evolve from a high scale Q towards lower values
- At a scale near Λ_{QCD}~200 MeV, perturbation theory breaks down and hadrons are formed
- Before that, at scales ~ few x Λ_{QCD}, there is universal preconfinement of colour
- Colour, flavour and momentum flows are only locally redistributed by hadronization



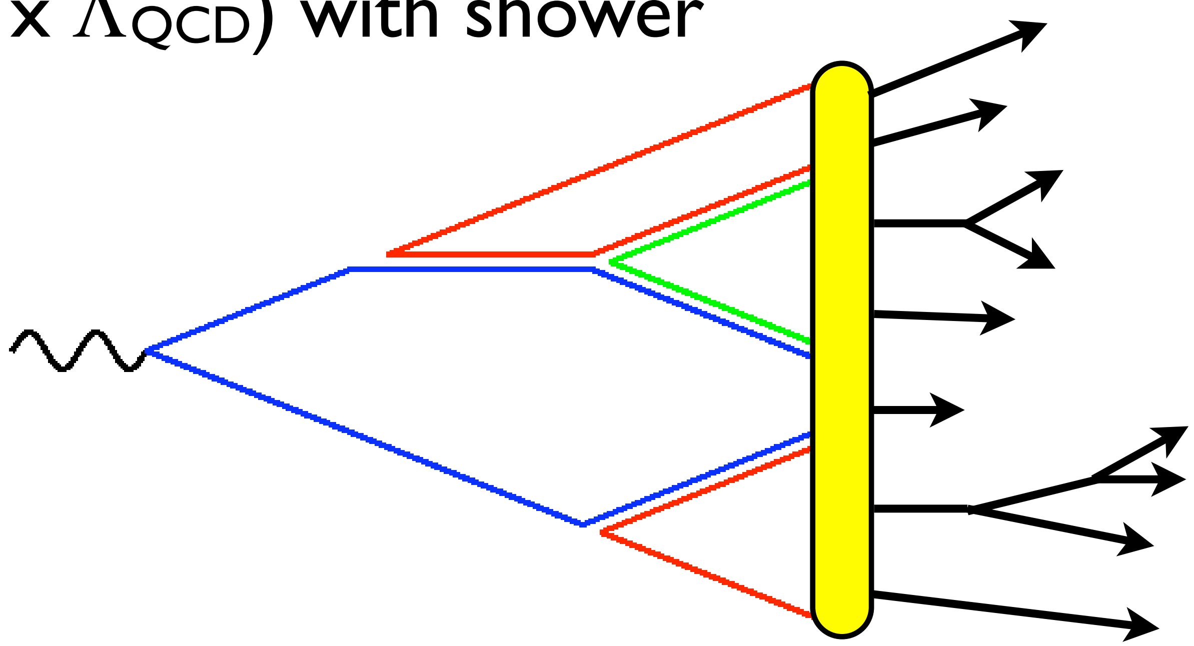
String Hadronization Model

- In parton shower, relative transverse momenta evolve from a high scale Q towards lower values
- At a scale near Λ_{QCD}~200 MeV, perturbation theory breaks down and hadrons are formed
- Before that, at scales ~ few x Λ_{QCD}, there is universal preconfinement of colour
- Colour flow dictates how to connect hadronic string (width ~ few x Λ_{QCD}) with shower



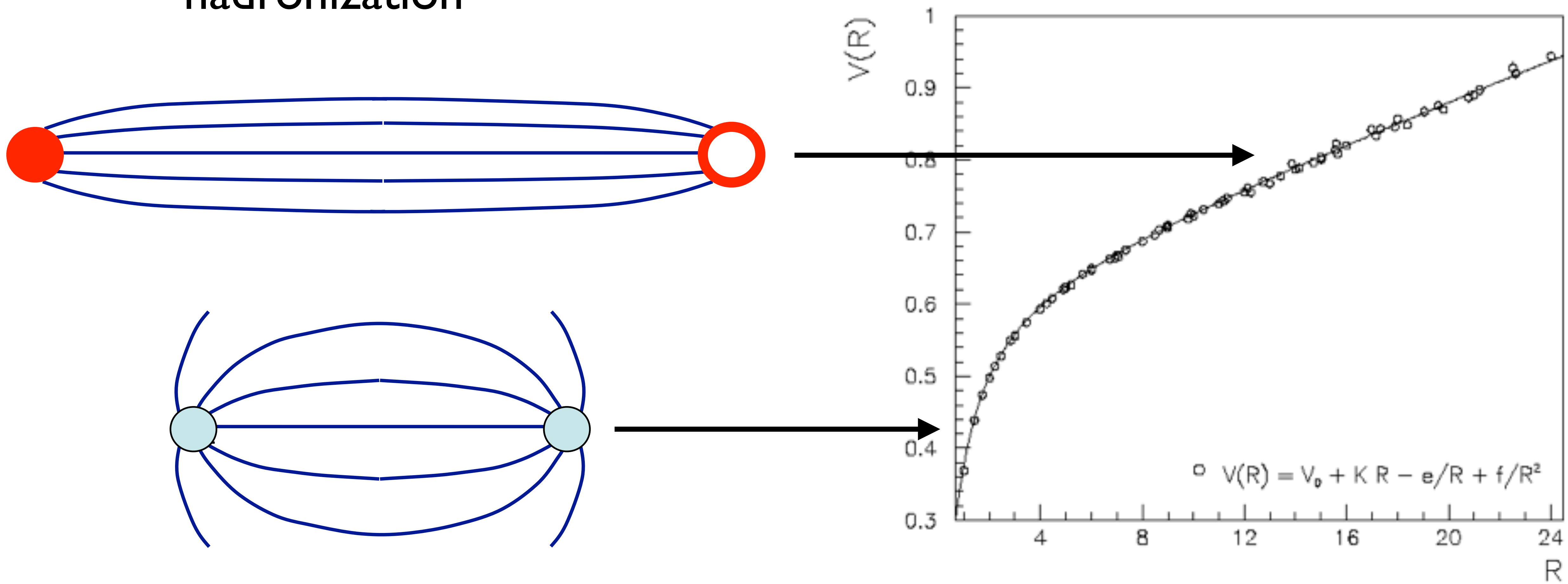
String Hadronization Model

- In parton shower, relative transverse momenta evolve from a high scale Q towards lower values
- At a scale near Λ_{QCD}~200 MeV, perturbation theory breaks down and hadrons are formed
- Before that, at scales ~ few x Λ_{QCD}, there is universal preconfinement of colour
- Colour flow dictates how to connect hadronic string (width ~ few x Λ_{QCD}) with shower



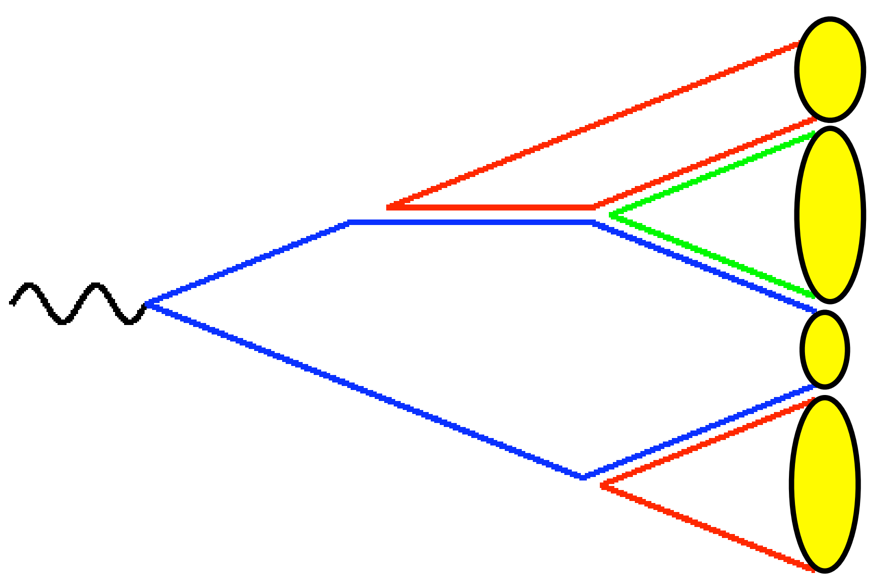
String Hadronization Model

- At short distances (large Q), QCD is like QED: colour field lines spread out (1/r potential)
- At long distances, gluon self-attraction gives rise to colour string (linear potential, quark confinement)
- Intense colour field induces quark-antiquark pair creation: hadronization



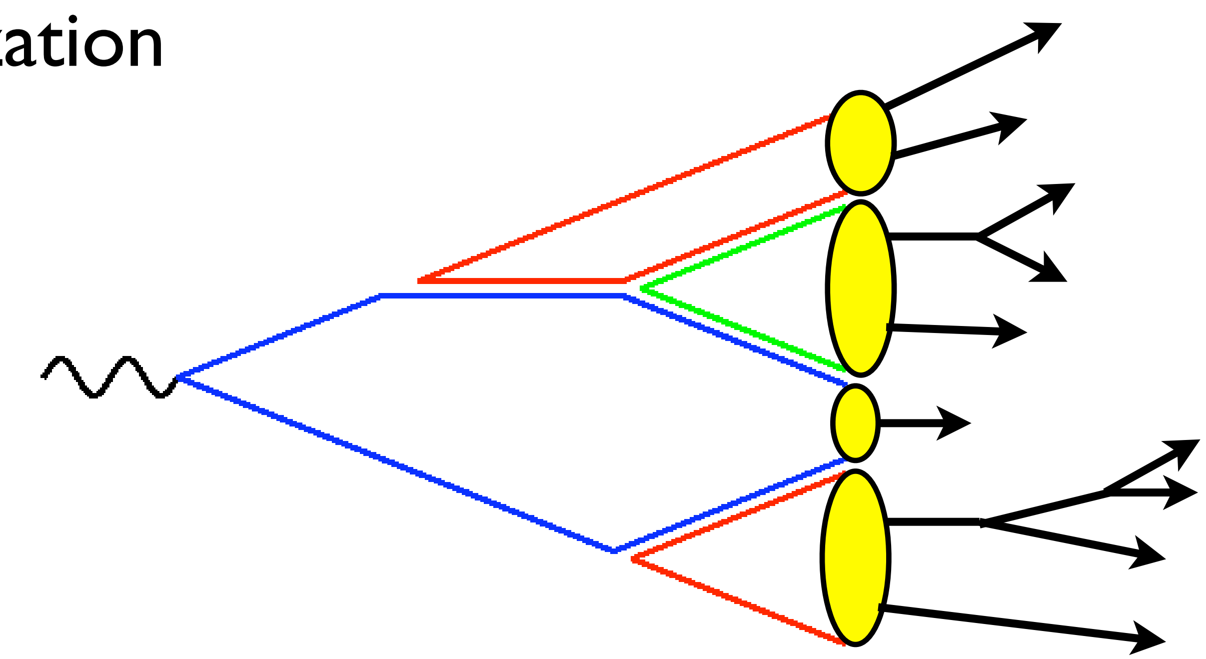
Cluster Hadronization Model

- In parton shower, relative transverse momenta evolve from a high scale Q towards lower values
- At a scale near Λ_{QCD}~200 MeV, perturbation theory breaks down and hadrons are formed
- Before that, at scales ~ few x Λ_{QCD}, there is universal preconfinement of colour
- Decay of preconfined clusters provides a direct basis for hadronization

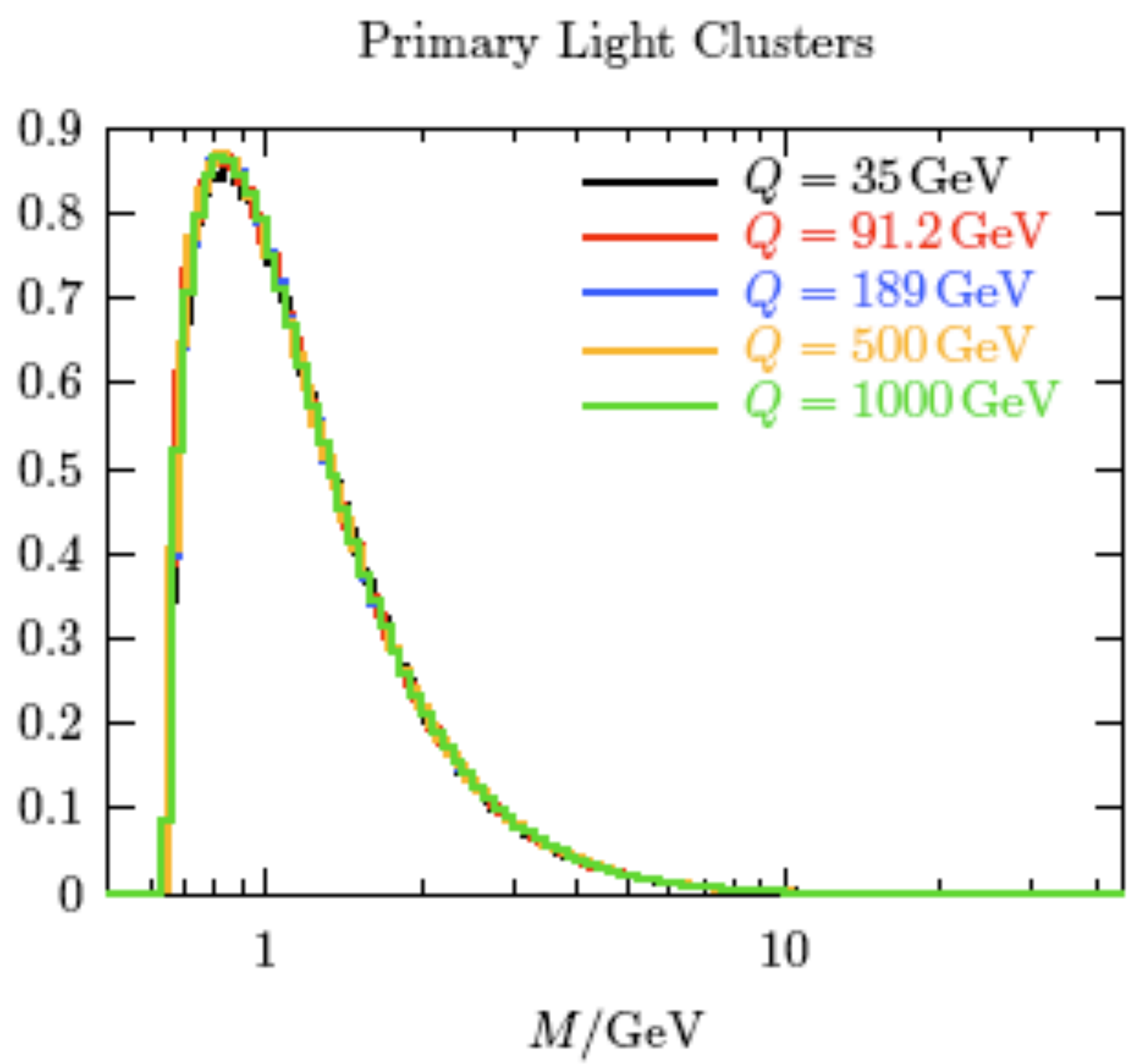


Cluster Hadronization Model

- In parton shower, relative transverse momenta evolve from a high scale Q towards lower values
- At a scale near Λ_{QCD}~200 MeV, perturbation theory breaks down and hadrons are formed
- Before that, at scales ~ few x Λ_{QCD}, there is universal preconfinement of colour
- Decay of preconfined clusters provides a direct basis for hadronization



Cluster Hadronization Model

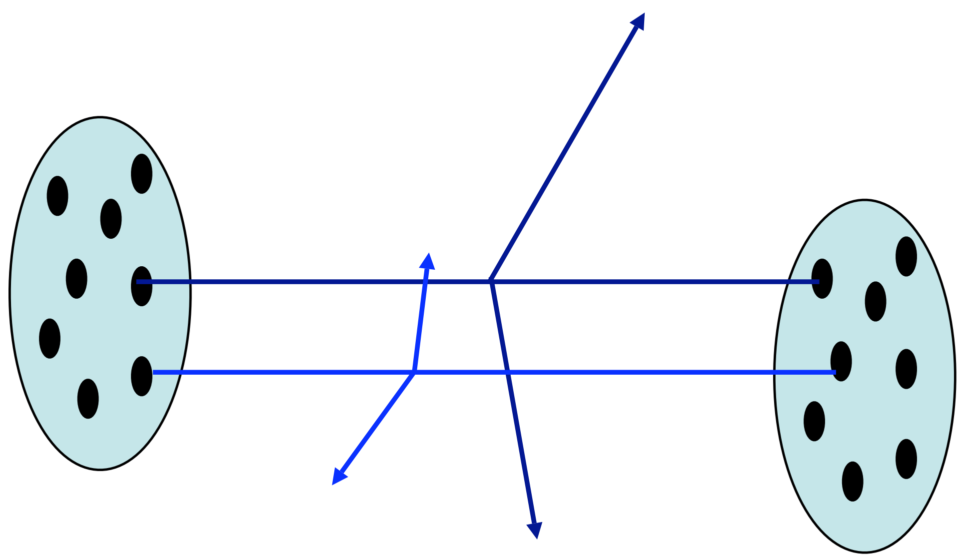


- Mass distribution of preconfined clusters is universal
- Phase-space decay model for most clusters
- High-mass tail decays anisotropically (string-like)

Hadronization Status

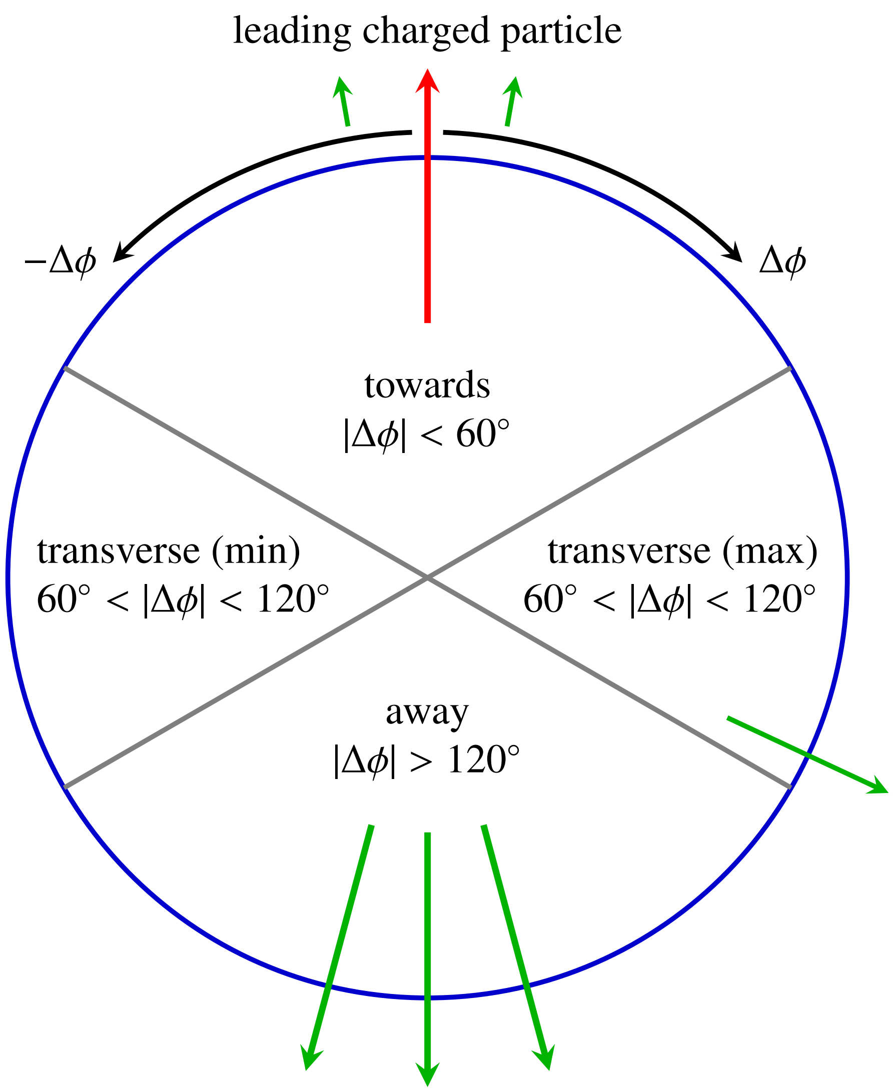
- No fundamental progress since 1980s
  - Available non-perturbative methods (lattice, AdS/QCD, ...) are not applicable
- Less important in some respects in LHC era
  - Jets, leptons and photons are observed objects, not hadrons
- But still important for detector effects
  - Jet response, heavy-flavour tagging, lepton and photon isolation, ...

Underlying Event (MPI)

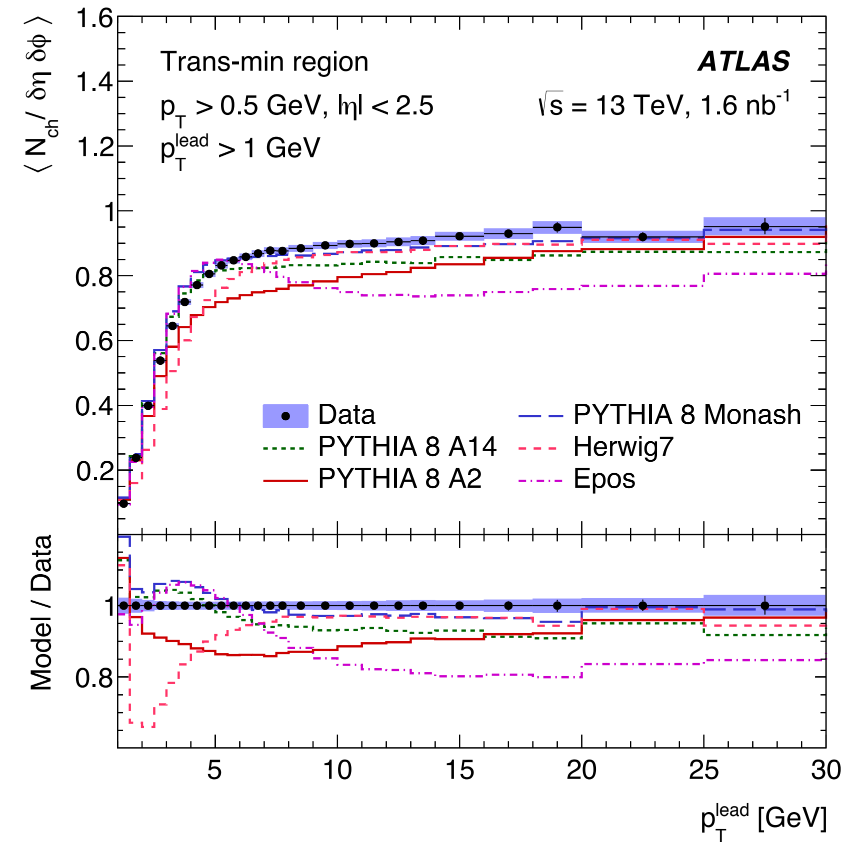


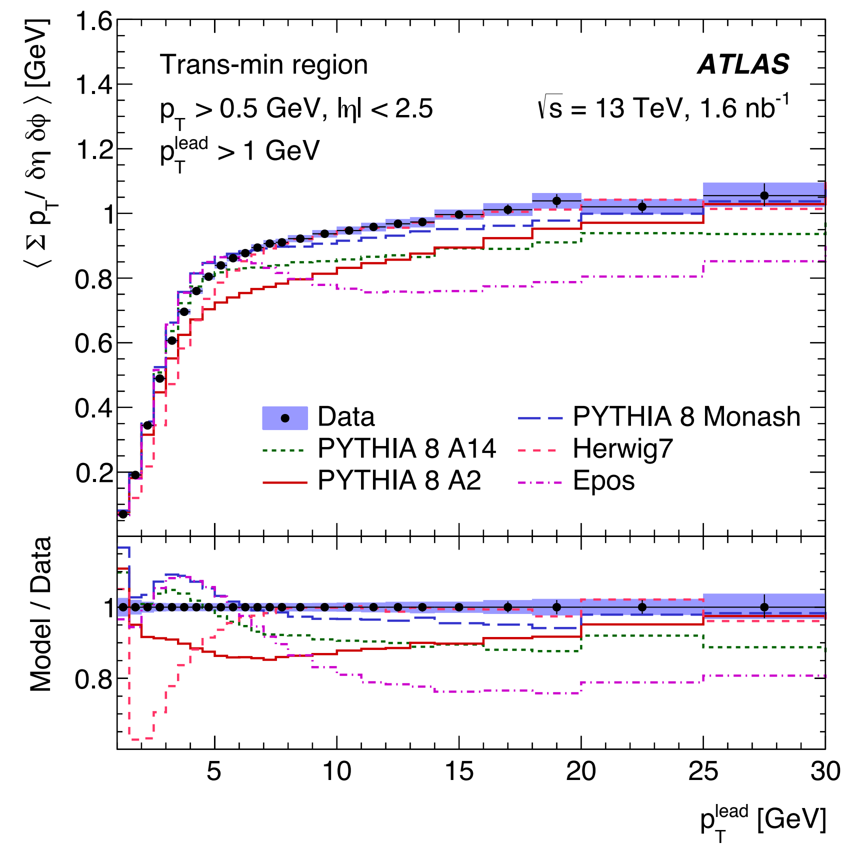
- Multiple parton interactions in same collision
  - Depends on density profile of proton
- Assume QCD 2-to-2 secondary collisions
  - Need cutoff at low p_T
- Need to model colour flow
  - Colour reconnections are necessary

Underlying Event

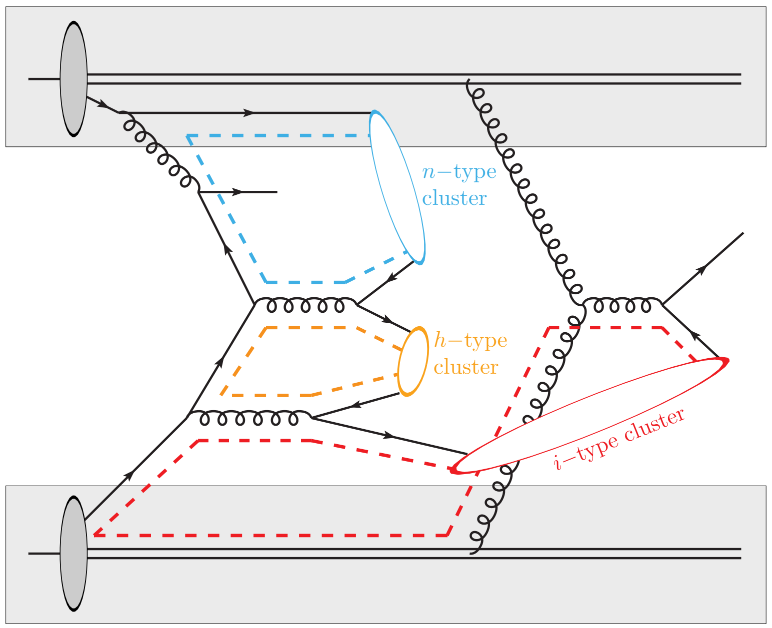


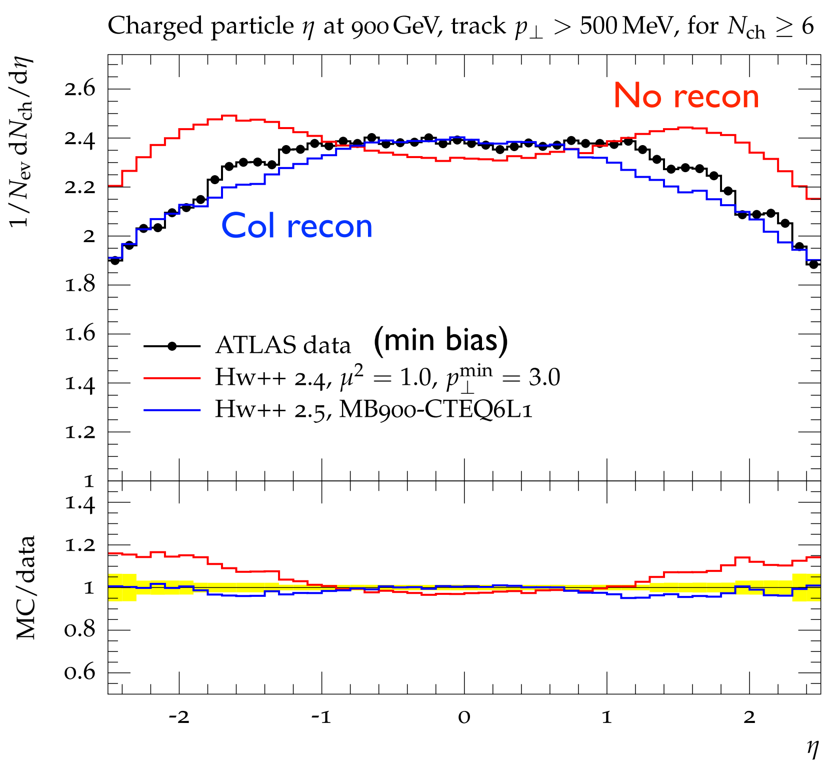
ATLAS, JHEP 03(2017)157

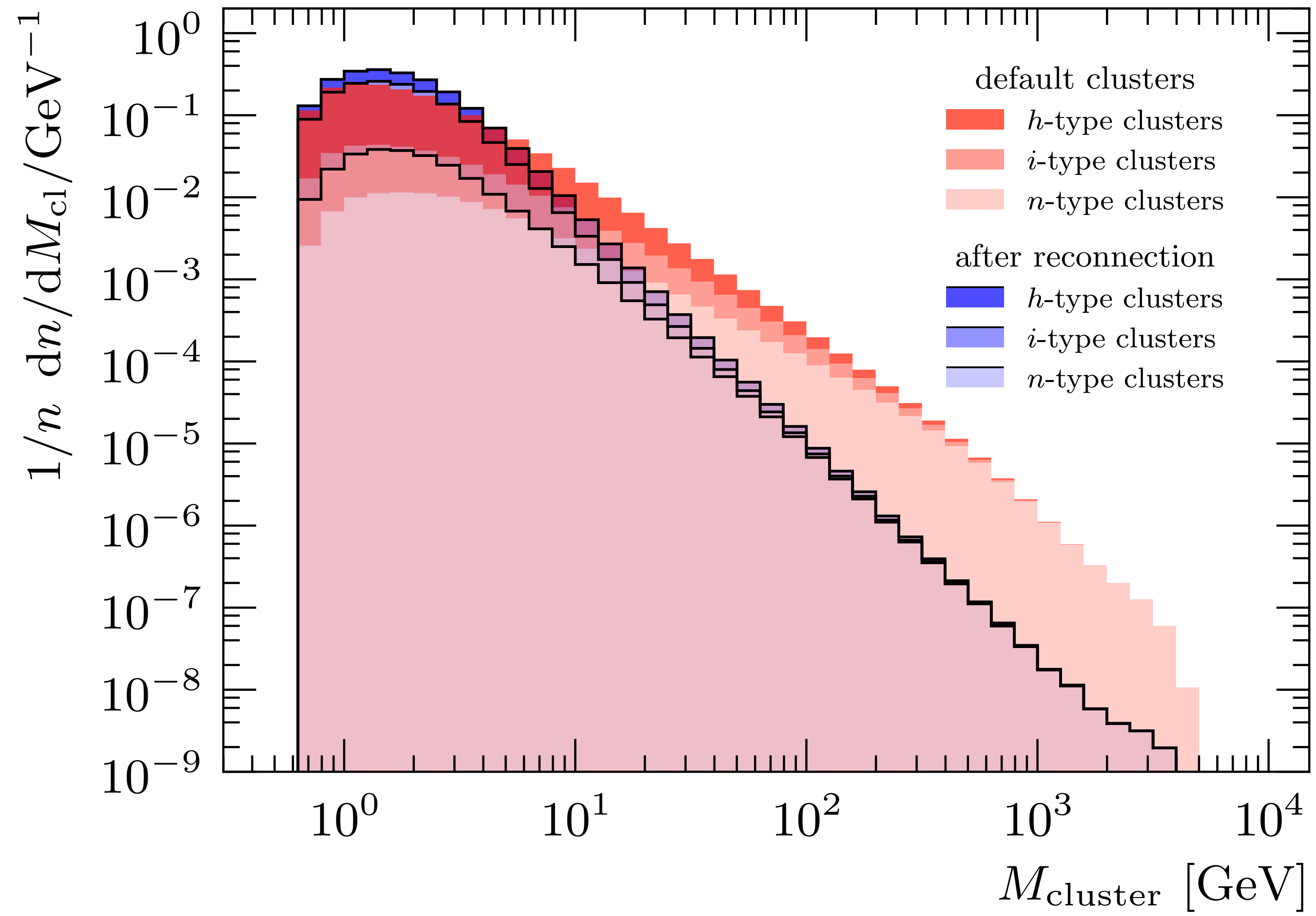




Colour Reconnection







- "Colour length" $\lambda \equiv \sum_{i=1}^{N_{cl}} m_i^2$ reduced by reconnection
- Massive leading clusters reduced
- Similar need in string model

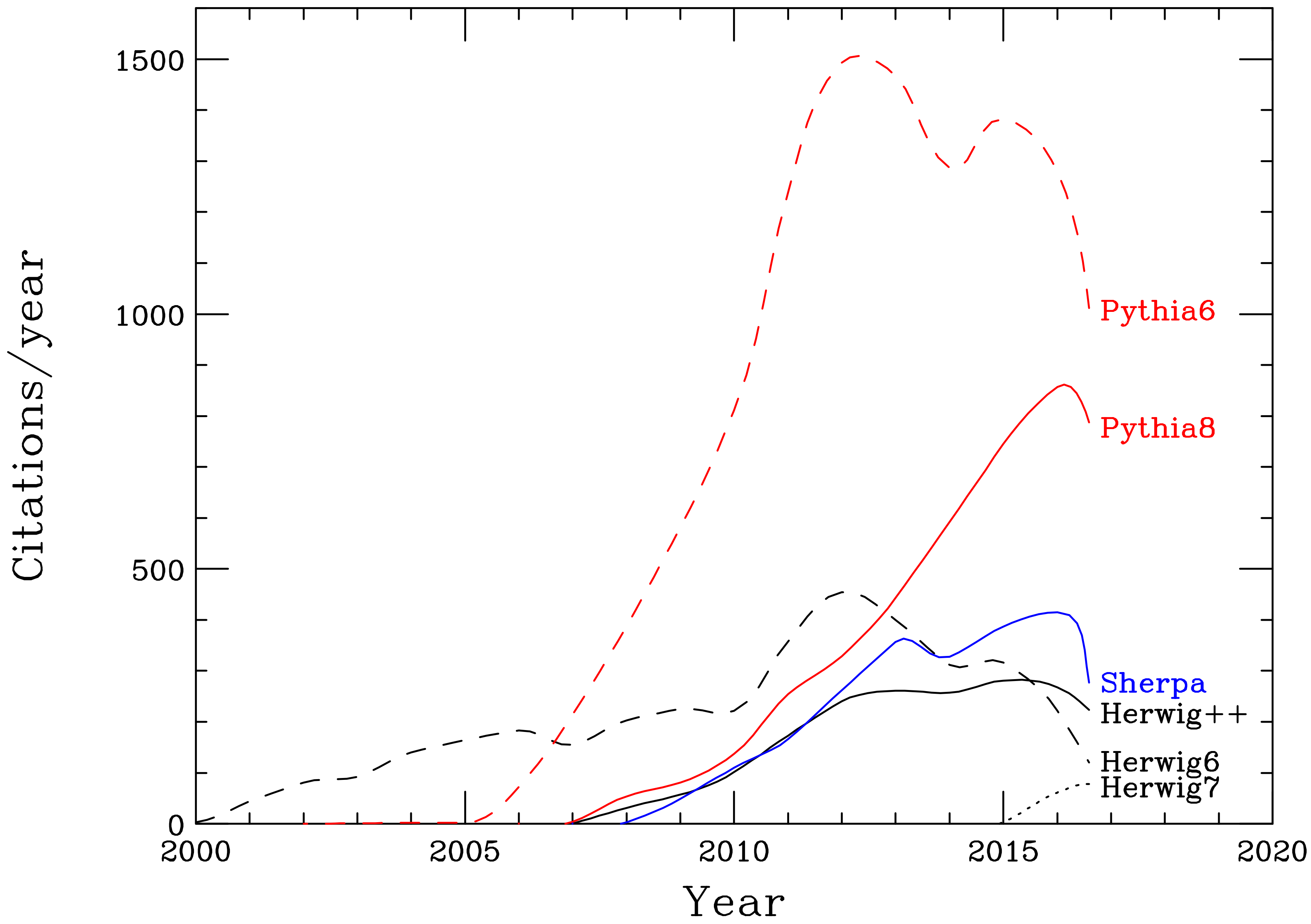
Gieseke, Röhr, Siódmok, EPJC72(2012)2225

Event Generators

- **HERWIG** http://projects.hepforge.org/herwig/
  - Angular-ordered parton shower, cluster hadronization
  - v6 Fortran; Herwig++
- **PYTHIA** http://www.thep.lu.se/~torbjorn/Pythia.html
  - Dipole-type parton shower, string hadronization
  - v6 Fortran; v8 C++
- **SHERPA** http://projects.hepforge.org/sherpa/
  - Dipole-type parton shower, cluster hadronization
  - C++

"General-purpose event generators for LHC physics",
A Buckley et al., arXiv:1101.2599, Phys. Rept. 504(2011)145

Generator Citations



- Most-cited article only for each version
- 2017 is extrapolation (Jan to July x12/7)

Other relevant software
(with apologies for omissions)

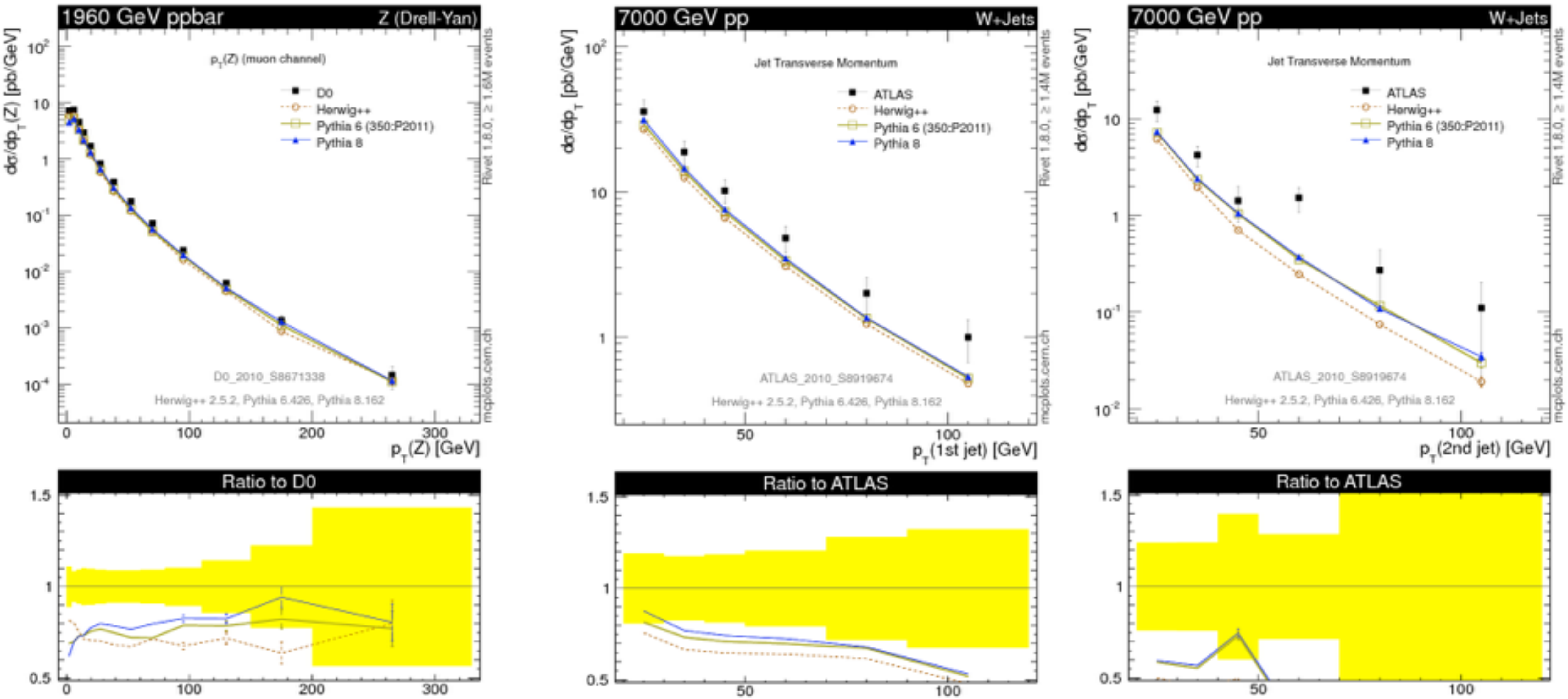
- Other event/shower generators: PhoJet, Ariadne, Dipsy, Cascade, Vincia
- Matrix-element generators: MadGraph/MadEvent, CompHep, CalcHep, Helac, Whizard, Sherpa, GoSam, aMC@NLO
- Matrix element libraries: AlpGen, POWHEG BOX, MCFM, NLOjet++, VBFNLO, BlackHat, Rocket
- Special BSM scenarios: Prospino, Charybdis, TrueNoir
- Mass spectra and decays: SOFTSUSY, SPHENO, HDecay, SDecay
- Feynman rule generators: FeynRules
- PDF libraries: LHAPDF
- Resummed ($p_\perp$) spectra: ResBos
- Approximate loops: LoopSim
- Jet finders: anti-$k_\perp$ and FastJet
- Analysis packages: Rivet, Professor, MCPLOTS
- Detector simulation: GEANT, Delphes
- Constraints (from cosmology etc): DarkSUSY, MicrOmegas
- Standards: PDF identity codes, LHA, LHEF, SLHA, Binoth LHA, HepMC

Sjöstrand, Nobel Symposium, May 2013

Parton Shower Monte Carlo

- Hard subprocess: $q\bar{q} \to Z^0/W^\pm$

http://mcplots.cern.ch/



- Leading-order (LO) normalization ➡ need next-to-LO (NLO)
- Worse for high p_T and/or extra jets ➡ need multijet merging

Summary on Event Generators

- Fairly good overall description of data, but…
- Hard subprocess: LO no longer adequate
- Parton showers: need matching to NLO
  - Also multijet merging
  - NLO showering?
- Hadronization: string and cluster models
  - Need new ideas/methods
- Underlying event due to multiple interactions
  - Colour reconnection necessary