### Monte Carlo simulations of hadronic collisions

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# **Factorization Theorem**

$$\frac{d\sigma}{dX} = \sum_{j,k} \int_{\hat{X}} f_j(x_1,Q_i) f_k(x_2,Q_i) \frac{d\hat{\sigma}_{jk}(Q_i,Q_f)}{d\hat{X}} F(\hat{X} \to X;Q_i,Q_f)$$



$$\hat{X} \rightarrow F \rightarrow X$$

$$f_j(x,Q)$$
 Parton distribution  
functions (PDF)

 sum over all initial state histories leading, at the scale Q, to:

$$\vec{p}_j = x \vec{P}_{proton}$$

$$F(\hat{X} \rightarrow X; Q_i, Q_f)$$

- transition from partonic final state to the hadronic observable (hadronization, fragm. function, jet definition, etc)
- Sum over all histories with X in them

- The possible histories of initial and final state, and their relative probabilities, are in principle independent of the hard process (they only depend on the flavours of partons involved and on the scales Q)
- Once an algorithm is developed to describe initial (IS) and final (FS) state evolution, it can be applied to partonic IS and FS arising from the calculation of an arbitrary hard process
- Depending on the extent to which different possible FS and IS histories affect the value of the observable X, different realizations of the factorization theorem can be implemented, and 3 different tools developed:
  - I. Cross-section evaluators
  - 2. Parton-level Monte Carlos
  - 3. Shower Monte Carlos

### I: Cross-section evaluators

- Only some component of the final state is singled out for the measurement, all the rest being ignored (i.e. integrated over). E.g.
   pp→e<sup>+</sup>e<sup>-</sup> + X
- No 'events' are 'generated', only cross-sections are evaluated:

$$\sigma(pp \rightarrow Z^0), \quad \frac{d\sigma}{dM(e^+e^-)\,dy(e^+e^-)}, \quad \dots$$

Experimental selection criteria (e.g. jet definition or acceptance) are applied on parton-level quantities. Provided these are infrared/ collinear finite, it therefore doesn't matter what  $\mathbf{F}(\mathbf{X})$  is, as we assume (*fact. theorem.*) that:  $\sum F(\hat{X}, X) = 1 \quad \forall \hat{X}$ 

X

### State of the art

- NLO available for:
  - jet and heavy quarks production
  - prompt photon production
  - gauge boson pairs
  - most new physics processes (e.g. SUSY)
- NNLO available for:
  - W/Z/DY production  $(q\bar{q} \rightarrow W)$
  - Higgs production  $(gg \rightarrow H)$

#### 2: Parton-level (aka matrix-element) MC's

- Parton level configurations (i.e. sets of quarks and gluons) are generated, with probability proportional to the respective perturbative M.E.
- Transition function between a final-state parton and the observed object (jet, missing energy, lepton, etc) is unity
- No need to expand f(x) or F(X) in terms of histories, since they all lead to the same observable
- Experimentally, equivalent to assuming
  - perfect jet reconstruction ( $\mathbf{P}_{\mu}^{parton} \rightarrow \mathbf{P}_{\mu}^{jet}$ )
  - linear detector response

### State of the art

- W/Z/gamma + N jets (N≤6)
- W/Z/gamma + Q Qbar + N jets (N≤4)
- Q Qbar + N jets (N≤4)
- Q Qbar Q' Q'bar + N jets (N≤2)
- Q Qbar H + N jets (N≤3)
- nW + mZ + kH + N jets ( $n+m+k+N \le 8, N\le 2$ )

■ N jets (N≤8)

Example of complexity of the calculations, for gg-> N gluons:

Njets	2	3	4	5	6	7	8
# diag's	4	25	220	2485	34300	5x10 <sup>5</sup>	10 <sup>7</sup>

For each process, flavour state and colour flow (leading I/Nc) are calculated on an eventby-event basis, to allow QCD-coherent shower evolution

ALPGEN: MLM, Moretti, Piccinini, Pittau, Polosa MADGRAPH: Maltoni, Stelzer CompHEP: Boos etal VECBOS: Giele et al NJETS: Giele et al Kleiss, Papadopoulos

.....

#### **3: Shower Monte Carlos**

# **Goal:** complete description of the event, at the level of individual hadrons



#### **Evolution of hadronic final states**

Asymptotic freedom implies that at  $E_{CM} >> I \text{ GeV}$ 

 $\sigma(e^+ e^- \rightarrow hadrons) \longrightarrow \sigma(e^+ e^- \rightarrow quarks/gluons)$ 

At the Leading Order (LO) in PT:



$$\sigma_0(e^+e^- \to q\bar{q}) = \frac{4\pi\alpha^2}{9s} N_c \sum_{f=u,d,\dots} e_q^2$$

$$\frac{\sigma_0(e^+e^- \to q\bar{q})}{\sigma_0(e^+e^- \to \mu^+\mu^-)} = N_c \sum_{f=u,d,\dots} e_{q_f}^2$$



$$\frac{\sigma_0(e^+e^- \to Z \to q\bar{q})}{\sigma_0(e^+e^- \to Z \to \mu^+\mu^-)} = N_c \frac{\sum_{f=u,d,\dots} \left(v_{q_f}^2 + a_{q_f}^2\right)}{\left(v_{\mu}^2 + a_{\mu}^2\right)}$$

Adding higher-order perturbative terms:

$$\sigma_1(e^+e^- \to q\bar{q}(g)) = \sigma_0(e^+e^- \to q\bar{q}) \left(1 + \frac{\alpha_s(E_{CM})}{\pi} + O(\alpha_s^2)\right)$$

O(3%) at M<sub>Z</sub>



# Excellent agreement with data, **provided N<sub>c</sub>=3**

Extraction of  $\alpha$ s consistent with the Q evolution predicted by QCD

Experimentally, the final states contain a large number of particles, not the 2 or 3 which apparently saturate the perturbative cross-section.



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#### Look more closely at the structure of these events:





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 $e^+ e^- \rightarrow qq \implies e^+ e^- \rightarrow 2 \text{ jets}$ 

$$e^+ e^- \rightarrow qqg \implies e^+ e^- \rightarrow 3$$
 jets

The puzzle is solved by associating partons to collimated "**jets**" of hadrons

#### **Angular ordering**



Radiation inside the cones is allowed, and described by the eikonal probability, radiation outside the cones is suppressed and averages to 0 when integrated over the full azimuth



2000 0000 0000 0000 0000

The construction can be iterated to the next emission, with the result that emission angles keep getting smaller and smaller => jet structure

Total colour charge of the system is equal to the quark colour charge. Treating the system as the incoherent superposition of N gluons would lead to artificial growth of gluon multiplicity. Angular ordering enforces coherence, and leads to the proper evolution with energy of particle multiplicities.



I: Generate the parton-level hard event



**II: Develop the parton shower** 



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I. Final state



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I. Final state

2. Initial state





I. Split gluons into q-qbar pairs



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- 2. Connect colour-singlet pairs



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V(d) ~ k d  $V(d_0) \sim 2 m_q$ . B= (qqq) B= ( qqq)

The structure of the perturbative evolution leads naturally to the clustering in phase-space of colour-singlet parton pairs ("preconfinement"). Long-range correlations are strongly suppressed. Hadronization will only act locally, on lowmass colour-singlet clusters.



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Colour is left "behind" by the struck quark. The first soft gluon emitted at large angle will connect to the beam fragments, ensuring that the beam fragments can recombine to form hadrons, and will allow the struck quark to evolve without having to worry about what happens to the proton fragments. 20



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a LLLL



Sequential probabilistic evolution (Markov chain)

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The total probability of all possible evolutions is **I** (unitary evolution).

- The shower evolution does not change the event rate inherited from the parton level, matrix element computation.
- No K-factors from the shower, even though the shower describes higher-order corrections to the leading-order process

## Single emission



 $\mathbf{q^2} \approx \text{virtuality scale of the branching:}$ 

**z=P(k<sub>2</sub>)/P(k)**≈ energy/ momentum fraction carried by one of the two partons after splitting

$$\frac{d\operatorname{Prob}(Q_0 \rightarrow q^2)}{dq^2 dz d\phi} = P_0 \frac{\alpha_s(\mu)}{2\pi} \frac{1}{q^2} P(z)$$
• (k\_1 + k\_2)<sup>2</sup>
• k\_1 • k\_2
• k\_{\perp}^2
• k\_{\perp}^2
• \dots
• P = k^0
• P = k / / + k^0
• \dots
• P = k / / + k^0
• \dots

While at leading-logarithmic order (LL) all choices of evolution variables and of scale for  $\alpha$ s are equivalent, specific choices can lead to improved description of NLL effects and allow a more accurate and easy-to-implement inclusion of angular-ordering constraints and mass effects, as well as to a better merging of multijet ME's with the shower

#### **Multiple emission**



$$2\pi JQ_1 q$$

$$\operatorname{Prob}(Q_0 \to Q_1 \to Q_2) = P_0 \frac{\alpha_s}{2\pi} \int_{Q_1}^{Q_0} \frac{dq^2}{q^2} dz P(z) d\phi \frac{\alpha_s}{2\pi} \int_{Q_2}^{Q_1} \frac{dq^2}{q^2} dz P(z) d\phi \\ \sim P_0 \frac{1}{2!} [\frac{\alpha_s}{2\pi} \int_{Q_2}^{Q_0} \frac{dq^2}{q^2} dz P(z) d\phi]^2$$

$$\operatorname{Prob}(Q_0 \to X) = P_0 \times \sum \frac{1}{n!} \left[\frac{\alpha_s}{2\pi} \int_{\Lambda}^{Q_0} \frac{dq^2}{q^2} dz P(z) d\phi\right]^n = 1 \qquad \Lambda = \text{infrared cutoff}$$

$$P_0 = \exp\{-\frac{\alpha_s}{2\pi}\int_{\Lambda}^{Q_0}\frac{dq^2}{q^2}dzP(z)d\phi\}$$

 $P_0$  = Sudakov form factor ~ probability of no emission between the scale  $Q_0$  and  $\Lambda$ 

### **Generation of splittings**

$$P(Q,\Lambda) = exp\left[-\int_{\Lambda}^{Q} \frac{dq^2}{q^2} \frac{\alpha_s(q)}{2\pi} P(z)dz\right]$$

prob. of no radiation between Q and  $\Lambda$ 



I.Generate  $0 < \xi_1 < 1$ 

2.If  $\xi_{I} < P(Q, \Lambda) \Rightarrow$  no radiation, q' goes directly on-shell at scale A≈GeV

3.Else

I.calculate Q<sub>1</sub> such that  $P(Q_1, \Lambda) = \xi_1$ 

2.emission at scale  $Q_{12}$ 



4.Select z according to P(z)

- 5.Reconstruct the full kinematics of the splitting
- 6.Go back to 1) and reiterate, until shower stops in 2). At each step the probability of emission gets smaller and smaller



The existence of high-mass clusters, however rare, is unavoidable, due to IR cutoff which leads to a non-zero probability that no emission takes place. This is particularly true for evolution of massive quarks (as in, e.g.  $Z \rightarrow bb$  or cc). Prescriptions have to be defined to deal with the "evolution" of these clusters. This has an impact on the  $z \rightarrow i$  behaviour of fragmentation functions.

Phenomenologically, this leads to uncertainties, for example, in the background rates for  $H \rightarrow \gamma \gamma$  (jet  $\rightarrow \gamma$ ). 25

This approach is extremely	Particle	Experiment	Measured	Old Model	Herwig++	Fortran
anossaful in desembing the	All Charged	M,A,D,L,O	$20.924 \pm 0.117$	$20.22^{*}$	20.814	$20.532^{*}$
successful in describing the	γ	A,O	$21.27 \pm 0.6$	23.03	22.67	20.74
properties of hadronic final states!	$\pi^0$	A,D,L,O	$9.59\pm0.33$	10.27	10.08	9.88
	$\rho(770)^{0}$	A,D	$1.295\pm0.125$	1.235	1.316	1.07
	$\pi^{\pm}$	A,O	$17.04\pm0.25$	16.30	16.95	16.74
	$\rho(770)^{\pm}$	0	$2.4\pm0.43$	1.99	2.14	2.06
	η	A,L,O	$0.956\pm0.049$	0.886	0.893	$0.669^{*}$
	$\omega(782)$	A,L,O	$1.083\pm0.088$	0.859	0.916	1.044
Ex: Particle multiplicities:	$\eta'(958)$	A,L,O	$0.152 \pm 0.03$	0.13	0.136	0.106
	$K^0$	S,A,D,L,O	$2.027\pm0.025$	$2.121^{*}$	2.062	2.026
	$K^{*}(892)^{0}$	A,D,O	$0.761\pm0.032$	0.667	0.681	$0.583^{*}$
	$K^{*}(1430)^{0}$	D,O	$0.106\pm0.06$	0.065	0.079	0.072
	$K^{\pm}$	A,D,O	$2.319\pm0.079$	2.335	2.286	2.250
	$K^{*}(892)^{\pm}$	A,D,O	$0.731\pm0.058$	0.637	0.657	0.578
	$\phi(1020)$	A,D,O	$0.097\pm0.007$	0.107	0.114	$0.134^{*}$
	p	A,D,O	$0.991\pm0.054$	0.981	0.947	1.027
	$\Delta^{++}$	D,O	$0.088\pm0.034$	0.185	0.092	$0.209^{*}$
	$\Sigma^{-}$	0	$0.083\pm0.011$	0.063	0.071	0.071
	1	A,D,L,O	$0.373\pm0.008$	$0.325^{*}$	0.384	$0.347^{*}$
Table 2: Multiplicities per event at 91.2 GeV. We show results from Herwig++ with th	e 10	A,D,O	$0.074\pm0.009$	0.078	0.091	0.063
(Harris 1.1) and from HEDWIC 6.5 channels and be descination (Extern). Depute	a 1+	0	$0.099\pm0.015$	0.067	0.077	0.088
(Herwig++), and from HERWIG 0.5 shower and nadronization (Fortran). Parameter values used are given in table 1. Experiments are Alexh(A). Delphi(D), 12(L). Opel(O)	$(1385)^{\pm}$	A,D,O	$0.0471\pm0.0046$	0.057	$0.0312^{*}$	$0.061^{*}$
whiles used are given in case 1. Experiments are Alepu( $A$ ), Depu( $D$ ), Es( $D$ ), Opa( $O$ ) Mk2( $M$ ) and SLD(S). The s indicates a prediction that differs from the measured value b	1-	A,D,O	$0.0262\pm0.001$	0.024	0.0286	0.029
more than three standard deviations.	$(1530)^0$	A,D,O	$0.0058\pm0.001$	$0.026^{*}$	$0.0288^{*}$	$0.009^{*}$
	_ <u>2</u> -	A,D,O	$0.00125\pm0.00024$	0.001	0.00144	0.0009
	$f_2(1270)$	D,L,O	$0.168\pm0.021$	0.113	0.150	0.173
	$f'_2(1525)$	D	$0.02 \pm 0.008$	0.003	0.012	0.012
	$D^{\pm}$	A,D,O	$0.184 \pm 0.018$	$0.322^{*}$	$0.319^{*}$	$0.283^{*}$
	$D^{*}(2010)^{\pm}$	A,D,O	$0.182\pm0.009$	0.168	0.180	$0.151^{*}$
	$D^0$	A,D,O	$0.473 \pm 0.026$	$0.625^{*}$	$0.570^{*}$	0.501
	$D_s^{\pm}$	A,O	$0.129\pm0.013$	$0.218^{*}$	$0.195^{*}$	0.127
	$D_s^{*\pm}$	0	$0.096\pm0.046$	0.082	0.066	0.043
	$J/\Psi$	A,D,L,O	$0.00544\pm0.00029$	0.006	$0.00361^{*}$	$0.002^{*}$
	$\Lambda_c^+$	D,O	$0.077\pm0.016$	$0.006^{*}$	$0.023^{*}$	$0.001^{*}$
	$\Psi'(3685)^{6}$	D.L.O	$0.00229 \pm 0.00041$	0.001*	0.00178	$0.0008^{*}$

#### **Ex: Energy distributions**

(Winter, Krauss, Soff, hep-ph/0311085)



#### Ex: Transverse momenta w.r.t. thrust axis:



#### Main limitation of shower approach:

Because of angular ordering



#### no emission outside $C_1 \oplus C_2$ :

lack of hard, large-angle emission
poor description of multijet events

#### incoherent emission inside $C_1 \oplus C_2$ :

Ioss of accuracy for intrajet radiation

#### Example



The obvious solution is to start the shower from a higher-order process calculated at the parton level with the exact LO matrix element:



Each hard parton then undergoes the shower evolution according to the previous prescription.

#### This approach is also afflicted by difficulties:



 $\Rightarrow$  double counting of the same phase-space points

Recent work started providing solutions to these problems, and new generations of MC codes successfully combine higher-order ME and shower evolution ("CKKW", "MLM matching")

## A useful ref:

# Hard Interactions of Quarks and Gluons: a Primer for LHC Physics

http://arXiv.org/abs/hep-ph/0611148