PYTHIA and other MC generators for pp physics

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The structure of an event

An event consists of many different physics steps to be modelled:
Signs of QGP-like collective behaviour in pp actively studied, but beyond default behaviour of standard pp generators.
The pp workhorses

**PYTHIA** (successor to JETSET, begun in 1978) originated in string hadronization studies. Historically strong interest in soft physics: MPI, CR. **Angantyr** model for pA/AA: Leif Lönnblad next.

**Herwig** (successor to EARWIG, begun in 1984) originated with coherent showers (angular ordering). MPI, CR and cluster hadronization added. Only simple event stacking for pA/AA.

**Sherpa** (APACIC++/AMEGIC++, begun in 2000) originated with matrix elements calculations. Emphasis on (N)NLO match & merge, less on soft. Heavy-ion effort under way (JEWEL, SHRIIMPS, ...).
PYTHIA core processes

Some (leading-order) processes hardcoded, almost freely mixable:

- **Soft QCD**: elastic, single diffractive, double diffractive, central diffractive, nondiffractive (including hard processes)
- **Hard QCD**: $2 \to 2$ (e.g. $qg \to qg$), open heavy flavours, charmonium, bottomonium, top, $(2 \to 3)$
- **Electroweak**: $f\bar{f} \to \gamma^*/Z^0$, $f\bar{f} \to W^+W^-$, $qg \to q\gamma$, $f\bar{f} \to \gamma\gamma$, $\ell q \to \ell q$, $q\gamma \to qg$, $\gamma\gamma \to f\bar{f}$, ...
- **Higgs** in the SM and various extensions
- **BSM**: SUSY, new gauge bosons, left–right symmetry, leptoquarks, compositeness, hidden valleys, extra dimensions, dark matter

**Other processes**: external input possible and common (LHA).

**Higher orders**: see presentation by Stefan Prestel; parton showers offer important complement.

**Sherpa and Herwig** have tighter integration of NLO than PYTHIA.
The Parton-Shower Approach

\[ 2 \rightarrow n = (2 \rightarrow 2) \oplus \text{ISR} \oplus \text{FSR} \]

ISR = Initial-State Radiation = spacelike showers
\[ Q_i^2 \sim -m^2 > 0 \] increasing

FSR = Final-State Radiation = timelike shower
\[ Q_i^2 \sim m^2 > 0 \] decreasing

Nowadays predominantly \( Q^2 \approx p_{\perp}^2 \) for both ISR and FSR.
Doublecounting

A $2 \rightarrow n$ graph can be “simplified” to $2 \rightarrow 2$ in different ways:

$g \rightarrow q\bar{q} \oplus qg \rightarrow qg$

or

$g \rightarrow gg \oplus gg \rightarrow q\bar{q}$

Do not doublecount: $2 \rightarrow 2 = $ most virtual = shortest distance
The DGLAP equations

### DGLAP (Dokshitzer–Gribov–Lipatov–Altarelli–Parisi)

\[
\begin{align*}
\frac{dP_{a \rightarrow bc}}{2\pi} &= \frac{\alpha_s}{Q^2} \frac{dQ^2}{Q^2} P_{a \rightarrow bc}(z) \, dz \\
\frac{P_{q \rightarrow qg}}{3} &= \frac{1 + z^2}{1 - z} \\
\frac{P_{g \rightarrow gg}}{3} &= \frac{(1 - z(1 - z))^2}{z(1 - z)} \\
\frac{P_{g \rightarrow q\bar{q}}}{2} &= n_f \left( z^2 + (1 - z)^2 \right) \quad (n_f = \text{no. of quark flavours})
\end{align*}
\]

**Universality:** any matrix element reduces to DGLAP in collinear limit.

**Example:**

\[
\frac{d\sigma(H^0 \rightarrow q\bar{q}g)}{d\sigma(H^0 \rightarrow q\bar{q})} = \frac{d\sigma(Z^0 \rightarrow q\bar{q}g)}{d\sigma(Z^0 \rightarrow q\bar{q})} \quad \text{in collinear limit}
\]
Radioactive decays and the Sudakov form factor

Naively $P(t) = c \implies N(t) = 1 - ct$. Wrong! Conservation of probability driven by depletion: a given nucleus can only decay once

Correctly

$P(t) = cN(t) \implies N(t) = \exp(-ct)$
i.e. exponential dampening

$P(t) = c \exp(-ct)$

Correspondingly, with $Q \sim 1/t$ (Heisenberg)

$$\frac{dP_{a \rightarrow bc}}{dz} = \frac{\alpha_s}{2\pi} \frac{dQ^2}{Q^2} P_{a \rightarrow bc}(z) \, dz$$

$$\times \exp \left( - \sum_{b',c'} \int_{Q^2}^{Q_{\text{max}}^2} \frac{dQ'^2}{Q'^2} \int \frac{\alpha_s}{2\pi} P_{a \rightarrow b'c'}(z') \, dz' \right)$$
If branching $a \rightarrow bc$, then $a$ reinterpreted from on-shell to off-shell. Not obvious how to conserve energy–momentum.

Dipole picture: a colour-connected parton $r$ takes the recoil, $p_b + p_c + p'_r = p_a + p_r$. Used iteratively. Lorentz invariant.

Not only a trick, but $a + r$ together define dipole/antenna with combined radiation pattern, well-defined in $N_C \rightarrow \infty$ limit.

Dipole showers available in all generators. For PYTHIA 3 options: default, and VINCIA and DIRE plugins. These differ by handling of ME corrections, $Q^2$ scales, etc. VINCIA and DIRE also include NLO branching kernels.

Herwig by default has an angular-ordered shower, with a post-facto rescaling of kinematics.
Matrix elements vs. parton showers

**ME : Matrix Elements**
+ systematic expansion in $\alpha_s$ (‘exact’)
+ powerful for multiparton Born level
+ flexible phase space cuts
− loop calculations very tough
− negative cross section in collinear regions
  ⇒ unpredictable jet/event structure
  − *no easy match to hadronization*

**PS : Parton Showers**
− approximate, to LL (or NLL)
− main topology not predetermined
+ process-generic ⇒ simple multiparton
+ Sudakov form factors/resummation
  ⇒ sensible jet/event structure
+ *easy to match to hadronization*

**Match & Merge:** consistently combine ME with PS.
The divergence of the QCD cross section

Cross section for $2 \rightarrow 2$ interactions is dominated by $t$-channel gluon exchange, so diverges like $\frac{d\hat{\sigma}}{dp_{\perp}^2} \approx \frac{1}{p_{\perp}^4}$ for $p_{\perp} \rightarrow 0$.

Integrate QCD $2 \rightarrow 2$

- $qq' \rightarrow qq'$
- $q\bar{q} \rightarrow q'\bar{q}'$
- $q\bar{q} \rightarrow gg$
- $qg \rightarrow qg$
- $gg \rightarrow gg$
- $gg \rightarrow q\bar{q}$

(with CTEQ 5L PDF's)
Hadrons are composite $\Rightarrow$ many partons can interact:

Divergence for $p_\perp \to 0$ in perturbative $2 \to 2$ scatterings;
tamed by unknown colour screening length $d$ in hadron

$$\frac{d\hat{\sigma}}{dp_\perp^2} \propto \frac{\alpha_s^2(p_\perp^2)}{p_\perp^4} \to \frac{\alpha_s^2(p_{\perp0}^2 + p_\perp^2)}{(p_{\perp0}^2 + p_\perp^2)^2}$$

with $p_{\perp0} \approx 2\text{–}3 \text{ GeV} \approx 1/d$.

Semiperturbative $2 \to 2$ generates whole nondiffractive $\sigma$!?
Hadrons are extended, so dependence on impact parameter $b$.

Overlap of protons during encounter is

$$O(b) = \int d^3x \, dt \, \rho_1(x, t) \rho_2(x, t)$$

where $\rho$ is (boosted) matter distribution in $p$, e.g. Gaussian or more narrow peak.

Average activity at $b$ proportional to $O(b)$:

- central collisions more active
  \[ \Rightarrow P_n \text{ broader than Poissonian}; \]
- peripheral passages normally give no collisions \( \Rightarrow \) finite $\sigma_{\text{tot}}$.

At LHC $\langle n_{\text{MPI}} \rangle \approx 3$ for all events, but $\gtrsim 10$ for central collisions.
Events with hard scale (jet, $W/Z$) have more underlying activity! Events with $n$ interactions have $n$ chances that one of them is hard, so “trigger bias”: hard scale $\Rightarrow$ central collision $\Rightarrow$ more interactions $\Rightarrow$ larger underlying activity.

Studied in particular by Rick Field, with CDF/CMS data:

- Define the MAX and MIN “transverse” regions on an event-by-event basis with MAX (MIN) having the largest (smallest) density.
Double Parton Scattering

\[ \sigma_{AB} = \frac{\sigma_A \sigma_B}{\sigma_{\text{eff}}} \]
\[ \sigma_{AA} = \frac{\sigma_A^2}{2 \sigma_{\text{eff}}} \]

State-of-the-art measurements

Experiment (energy, final state, year)

ATLAS
AFS (\(\sqrt{s} = 63\) GeV, 4 jets, 1986)
UA2 (\(\sqrt{s} = 630\) GeV, 4 jets, 1991)
CDF (\(\sqrt{s} = 1.8\) TeV, 4 jets, 1993)
CDF (\(\sqrt{s} = 1.8\) TeV, \(\gamma + 3\) jets, 1997)
DO (\(\sqrt{s} = 1.96\) TeV, \(\gamma + 3\) jets, 2010)
LHCb (\(\sqrt{s} = 7\) TeV, \(J/\psi\Lambda_c^+\), 2012)
LHCb (\(\sqrt{s} = 7\) TeV, \(J/\psi\Lambda^+\), 2012)
LHCb (\(\sqrt{s} = 7\) TeV, \(J/\psi\Lambda_c^+\), 2012)
LHCb (\(\sqrt{s} = 7\) TeV, \(J/\psi D^0\), 2012)
LHCb (\(\sqrt{s} = 7\) TeV, \(J/\psi\), 2012)
ATLAS (\(\sqrt{s} = 7\) TeV, \(W + 2\) jets, 2013)
CMS (\(\sqrt{s} = 7\) TeV, \(W + 2\) jets, 2014)
DO (\(\sqrt{s} = 1.96\) TeV, \(\gamma + b/c + 2\) jets, 2014)
DO (\(\sqrt{s} = 1.96\) TeV, \(\gamma + 3\) jets, 2014)
DO (\(\sqrt{s} = 1.96\) TeV, \(J/\psi + J/\psi\), 2014)
ATLAS (\(\sqrt{s} = 8\) TeV, \(Z + J/\psi\), 2015)
LHCb (\(\sqrt{s} = 7\)\&\(8\) TeV, \(Y(1S)D^{0,\pm}\), 2015)
DO (\(\sqrt{s} = 1.96\) TeV, \(J/\psi + Y\), 2016)
DO (\(\sqrt{s} = 1.96\) TeV, \(2\gamma + 2\) jets, 2016)
ATLAS (\(\sqrt{s} = 7\) TeV, 4 jets, 2016)
ATLAS (\(\sqrt{s} = 8\) TeV, \(J/\psi + J/\psi\), 2017)
CMS (\(\sqrt{s} = 8\) TeV, \(Y + Y\), 2017)
LHCb (\(\sqrt{s} = 13\) TeV, \(J/\psi + J/\psi\), 2017)
CMS (\(\sqrt{s} = 8\) TeV, \(W^+W^-\), 2018)
ATLAS (\(\sqrt{s} = 8\) TeV, 4 leptons, 2018)

\[ \sigma_{\text{eff}} [\text{mb}] \]

\[ \text{Dependence on c.m energy} \]

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Colour (re)connections and $\langle p_\perp \rangle(n_{\text{ch}})$

$\langle p_\perp \rangle(n_{\text{ch}})$ is very sensitive to colour flow

long strings to remnants $\Rightarrow$ much $n_{\text{ch}}$/interaction $\Rightarrow$ $\langle p_\perp \rangle(n_{\text{ch}}) \sim$ flat

short strings (more central) $\Rightarrow$ less $n_{\text{ch}}$/interaction $\Rightarrow$ $\langle p_\perp \rangle(n_{\text{ch}})$ rising

$n_{\text{ch}} \geq 1, p_T > 500$ MeV, $|\eta| < 0.8$
$\tau > 300$ ps
*ATLAS* $\sqrt{s} = 13$ TeV
At LEP 2 search for effects in $e^+e^- \rightarrow W^+W^- \rightarrow q_1\bar{q}_2 q_3\bar{q}_4$:

- **perturbative** $\langle \delta M_W \rangle \lesssim 5$ MeV: negligible!
- **nonperturbative** $\langle \delta M_W \rangle \sim 40$ MeV:
  
  **favoured**: no-effect option ruled out at 99.5% CL.

Best description for reconnection in $\approx 50\%$ of the events.

- **Bose-Einstein** $\langle \delta M_W \rangle \lesssim 100$ MeV: full effect ruled out (while models with $\sim 20$ MeV barely acceptable).
MPIs in PYTHIA

- MPIs are generated in a falling sequence of $p_{\perp}$ values; recall Sudakov factor approach to parton showers.
- Core process QCD $2 \rightarrow 2$, but also onia, $\gamma$’s, $Z^0$, $W^\pm$.
- Energy, momentum and flavour conserved step by step: subtracted from proton by all “previous” collisions.
- Protons modelled as extended objects, allowing both central and peripheral collisions, with more or less activity.
- Colour screening increases with energy, i.e. $p_{\perp 0} = p_{\perp 0}(E_{\text{cm}})$, as more and more partons can interact.
- Colour connections: each interaction hooks up with colours from beam remnants, but also correlations inside remnants.
- Colour reconnections: many interaction “on top of” each other $\Rightarrow$ tightly packed partons $\Rightarrow$ colour memory loss?
Interleaved evolution in PYTHIA

- Transverse-momentum-ordered parton showers for ISR and FSR
- MPI also ordered in $p_\perp$

$\Rightarrow$ Allows interleaved evolution for ISR, FSR and MPI:

$$
\frac{d\mathcal{P}}{dp_\perp} = \left( \frac{d\mathcal{P}_{\text{MPI}}}{dp_\perp} + \sum \frac{d\mathcal{P}_{\text{ISR}}}{dp_\perp} + \sum \frac{d\mathcal{P}_{\text{FSR}}}{dp_\perp} \right) \\
\times \exp \left( - \int_{p_\perp}^{p_{\perp\text{max}}} \left( \frac{d\mathcal{P}_{\text{MPI}}}{dp'_\perp} + \sum \frac{d\mathcal{P}_{\text{ISR}}}{dp'_\perp} + \sum \frac{d\mathcal{P}_{\text{FSR}}}{dp'_\perp} \right) dp'_\perp \right)
$$

Ordered in decreasing $p_\perp$ using “Sudakov” trick.
Corresponds to increasing “resolution”:
smaller $p_\perp$ fill in details of basic picture set at larger $p_\perp$.

- Start from fixed hard interaction $\Rightarrow$ underlying event
- No separate hard interaction $\Rightarrow$ minbias events
- Possible to choose two hard interactions, e.g. $W^-W^-$
Key point: two-component model

\[ p_\perp > p_\perp \text{min}: \text{pure perturbation theory (no modification)} \]
\[ p_\perp < p_\perp \text{min}: \text{pure nonperturbative ansatz} \]
- Number of MPIs first picked; then generated unordered in $p_\perp$.
- Interactions uncorrelated, up until energy used up.
- Force ISR to reconstruct back to gluon after first interaction.
- Impact parameter by em form factor shape, but tunable width.
- $p_{\perp \text{min}}$ scale to be tuned energy-by-energy.
- Colour reconnection essential to get $dn/d\eta$ correct.
The QCD string

QCD field lines compressed to tubelike region ⇒ string.
Gives linear confinement
\[ V(r) \approx \kappa r, \kappa \approx 1 \text{ GeV/fm}. \]
Confirmed e.g. on the lattice.

Nature of the string viewed in analogy with superconductors:

but QCD could be intermediate, or different.
String motion

The Lund Model: starting point

Use only linear potential \( V(r) \approx \kappa r \) to trace string motion, and let string fragment by repeated \( q\bar{q} \) breaks.

Assume negligibly small quark masses. Then linearity between space–time and energy–momentum gives

\[
\left| \frac{dE}{dz} \right| = \left| \frac{dp_z}{dz} \right| = \left| \frac{dE}{dt} \right| = \left| \frac{dp_z}{dt} \right| = \kappa
\]

\( (c = 1) \) for a \( q\bar{q} \) pair flying apart along the \( \pm z \) axis.
But signs relevant: the \( q \) moving in the \( +z \) direction has \( \frac{dz}{dt} = +1 \) but \( \frac{dp_z}{dt} = -\kappa \).
The Lund Model

Combine yo-yo-style string motion with string breakings!

Motion of quarks and antiquarks with intermediate string pieces:

- quark
- antiquark
- pair creation

A q from one string break combines with a \( \bar{q} \) from an adjacent one.

Gives simple but powerful picture of hadron production.
Where does the string break?

Fragmentation starts in the middle and spreads outwards:

Corresponds to roughly same invariant time of all breaks, 
\[ \tau^2 = t^2 - z^2 \sim \text{constant}, \]
with breaks separated by hadronic area \( m_\perp^2 = m^2 + p_\perp^2 \).

Hadrons at outskirts are more boosted.

Approximately flat rapidity distribution, \( \frac{dn}{dy} \approx \text{constant} \)
\[ \Rightarrow \text{total hadron multiplicity in a jet grows like } \ln E_{\text{jet}}. \]
How does the string break?

String breaking modelled by tunneling:

\[
P \propto \exp \left( -\frac{\pi m_{\perp}^2 q}{\kappa} \right) = \exp \left( -\frac{\pi p_{\perp}^2 q}{\kappa} \right) \exp \left( -\frac{\pi m_q^2}{\kappa} \right)
\]

- Common Gaussian \( p_{\perp} \) spectrum, \( \langle p_{\perp} \rangle \approx 0.4 \text{ GeV} \).
- Suppression of heavy quarks,
  \( u\bar{u} : d\bar{d} : s\bar{s} : c\bar{c} \approx 1 : 1 : 0.3 : 10^{-11} \).
- Diquark \( \sim \) antiquark \( \Rightarrow \) simple model for baryon production.

String model unpredictive in understanding of hadron mass effects
\( \Rightarrow \) many parameters, 10–20 depending on how you count.
The popcorn model for baryon production

- SU(6) (flavour × spin) Clebsch-Gordan's needed.
- Quadratic diquark mass dependence
  ⇒ strong suppression of multistrange and spin 3/2 baryons.
  ⇒ effective parameters with less strangeness suppression.
The Lund gluon picture

The most characteristic feature of the Lund model:

Gluon = kink on string

string motion in the event plane (without breakups)

Gluon = kink on string

Force ratio gluon/ quark = 2,
cf. QCD $N_C/C_F = 9/4$, $\rightarrow 2$ for $N_C \rightarrow \infty$

No new parameters introduced for gluon jets!
One Feynman graph can correspond to several possible colour flows, e.g. for $qg \rightarrow qg$:

while other $qg \rightarrow qg$ graphs only admit one colour flow:

Interference terms with indeterminate colour flow $\propto \frac{1}{N_C^2}$.
The Herwig cluster model

1. Force $g \rightarrow q\bar{q}$ branchings.
2. Form colour singlet clusters.
3. Decay high-mass clusters to smaller clusters.
4. Decay clusters to 2 hadrons according to phase space times spin weight.
5. New: allow three aligned $q\bar{q}$ clusters to reconnect to two clusters $q_1q_2q_3$ and $\bar{q}_1\bar{q}_2\bar{q}_3$.
6. New: allow nonperturbative $g \rightarrow s\bar{s}$ in addition to $g \rightarrow u\bar{u}$ and $g \rightarrow d\bar{d}$.
Herwig cluster model improvement

\[ \frac{K}{\pi} \text{ in INEL pp collisions at } \sqrt{s} = 7 \text{ TeV in } |y| < 0.5. \]

\[ \frac{p}{\pi} \text{ in INEL pp collisions at } \sqrt{s} = 7 \text{ TeV in } |y| < 0.5. \]

Gieseke, Kirchgaeßer, Plätzer, EPJ C78 (2018) 99
### String vs. Cluster

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The result for the total hadronic cross section presented here, $\sigma_{\text{tot}} = 9.35 \pm 1.36 \text{ mb}$, can be compared to the value measured by TOTEM in the same LHC fill using a luminosity-dependent analysis, $\sigma_{\text{tot}} = 9.86 \pm 2.2 \text{ mb}$\textsuperscript{[11]}. Assuming the uncertainties are uncorrelated, the difference between the ATLAS and TOTEM values corresponds to 1.3$\sigma$. The uncertainty on the TOTEM result is dominated by the luminosity uncertainty of $\pm 4\%$, while the measurement reported here profits from a smaller luminosity uncertainty of only $\pm 2.3\%$. In subsequent publications\textsuperscript{[16, 54]} TOTEM has used the same data set to perform a luminosity-independent measurement of the total cross section using a simultaneous determination of elastic and inelastic event yields. In addition, TOTEM made a $\rho$-independent measurement without using the optical theorem by summing directly the elastic and inelastic cross sections\textsuperscript{[16]}. The three TOTEM results are consistent with one another.

The results presented here are compared in Fig. 19 to the result of TOTEM and are also compared with results of experiments at lower energy\textsuperscript{[29]} and with cosmic ray experiments\textsuperscript{[55–58]}. The measured total cross section is furthermore compared to the best fit to the energy evolution of the total cross section from the COMPETE Collaboration\textsuperscript{[26]} assuming an energy dependence of $\ln s$. The elastic measurement is in turn compared to a second order polynomial fit in $\ln s$ of the elastic cross sections. The value of $\sigma_{\text{tot}}$ reported here is two standard deviations below the COMPETE parameterization. Some other models prefer a somewhat slower increase of the total cross section with energy, predicting values below 95 mb, and thus agree slightly better with the result reported here\textsuperscript{[59–61]}.
Ingelman-Schlein: Pomeron as hadron with partonic content

Diffractive event = (Pomeron flux) \times (pPp collision)

1) \sigma_{SD}, \sigma_{DD} and \sigma_{CD} set by Reggeon theory.
2) \text{f}_{IP/P}(x_{IP}, t) \Rightarrow \text{diffractive mass spectrum, } p_{\perp} \text{ of proton out.}
3) Smooth transition from simple model at low masses to IPp with full pp machinery: multiparton interactions, parton showers, etc.
4) Choice between different Pomeron PDFs.
5) Free parameter \sigma_{IPp} needed to fix \langle n_{\text{interactions}} \rangle = \sigma_{\text{jet}}/\sigma_{IPp}.
Multiplicity in diffractive events

$4 < \Delta \eta^F < 6$
$\sqrt{s} = 7$ TeV
$p_T > 200$ MeV

**ATLAS**

PYTHIA 6 lacks MPI, ISR, FSR in diffraction, so undershoots.
PYTHIA can calculate production vertex of each particle, e.g. number of hadrons as a function of time for pp at 13 TeV:

Hadronization process extends up to scales $E_{CM}/2 \kappa \approx 6000$ fm. Particle decays starts rapidly and then continues.
MCnet

Herwig
PYTHIA
Sherpa
MadGraph

Plugin:
Ariadne
DIPSY
HEJ

CEDAR:
Rivet
Professor
HepForge
LHAPDF
HepMC

- EU-funded 2007–10, 2013–16, **2017–21**
- Generator development
- Services to community
- PhD student training
- Common activities
- Summer schools
  - **2019: near London**
  - 2020: near Karlsruhe
- Short-term studentships
  (3 - 6 months).
  Formulate your project!
  Experimentalists welcome!

Nodes:
Manchester
Durham
Glasgow
Göttingen
Karlsruhe
UC London
Louvain
Lund
CERN
Heidelberg
Monash (Au)
Vienna

[https://www.montecarlonet.org/](https://www.montecarlonet.org/)
Summary and outlook

- Three main workhorses — PYTHIA, Herwig and Sherpa — allow for complementary model approaches and cross-checks.
- Publicly available and well supported, e.g. http://home.thep.lu.se/Pythia/
- (N)NLO calculations with match&merge to improved showers main development of latest 20 years.
- Multiparton interactions, colour reconnection and hadronization as important, but little to no deep theory, so often swept under the carpet.

Thank you!