

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:



Beyond current standard pp paradigm

I: Flavour composition



II: Flow

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, SHRiMPS, ...).

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: $2 \rightarrow 2$ (e.g. $qg \rightarrow qg$), open heavy flavours, charmonium, bottomonium, top, $(2 \rightarrow 3)$
- Electroweak: $f\bar{f} \rightarrow \gamma^*/Z^0$, $f\bar{f} \rightarrow W^+W^-$, $qg \rightarrow q\gamma$, $f\bar{f} \rightarrow \gamma\gamma$, $\ell q \rightarrow \ell q$, $q\gamma \rightarrow qg$, $\gamma\gamma \rightarrow f\bar{f}$, ...
- 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



$$\begin{split} &\text{ISR} = \text{Initial-State Radiation} = \text{spacelike showers} \\ &Q_i^2 \sim -m^2 > 0 \text{ increasing} \\ &\text{FSR} = \text{Final-State Radiation} = \text{timelike shower} \\ &Q_i^2 \sim m^2 > 0 \text{ decreasing} \\ &\text{Nowadays predominantly } Q^2 \approx p_1^2 \text{ for both ISR and FSR.} \end{split}$$

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A 2 \rightarrow *n* graph can be "simplified" to 2 \rightarrow 2 in different ways:



The DGLAP equations

DGLAP (Dokshitzer-Gribov-Lipatov-Altarelli-Parisi)

$$d\mathcal{P}_{a \to bc} = \frac{\alpha_s}{2\pi} \frac{dQ^2}{Q^2} P_{a \to bc}(z) dz$$

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

$$P_{g \to qg} = 3 \frac{(1-z(1-z))^2}{z(1-z)}$$

$$P_{g \to q\overline{q}} = \frac{n_f}{2} (z^2 + (1-z)^2) \quad (n_f = \text{no. of quark flavours})$$

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

e.g.
$$\frac{\mathrm{d}\sigma(\mathrm{H}^{0}\to\mathrm{q}\overline{\mathrm{q}}\mathrm{g})}{\mathrm{d}\sigma(\mathrm{H}^{0}\to\mathrm{q}\overline{\mathrm{q}})} = \frac{\mathrm{d}\sigma(\mathrm{Z}^{0}\to\mathrm{q}\overline{\mathrm{q}}\mathrm{g})}{\mathrm{d}\sigma(\mathrm{Z}^{0}\to\mathrm{q}\overline{\mathrm{q}})} \quad \mathrm{in \ collinear \ limit}$$

Radioactive decays and the Sudakov form factor

N(t) N_{0} N_{0}

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

$$d\mathcal{P}_{a \to bc} = \frac{\alpha_{s}}{2\pi} \frac{dQ^{2}}{Q^{2}} P_{a \to bc}(z) dz$$
$$\times \exp\left(-\sum_{b',c'} \int_{Q^{2}}^{Q_{\max}^{2}} \frac{dQ'^{2}}{Q'^{2}} \int \frac{\alpha_{s}}{2\pi} P_{a \to b'c'}(z') dz'\right)$$

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 $N_{\rm C} \rightarrow \infty$ 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 $\alpha_{\rm s}$ ('exact')
- + powerful for multiparton Born level
- + flexible phase space cuts
- loop calculations very tough
- $\begin{array}{ll} & {\rm negative\ cross\ section\ in\ collinear\ regions} \\ \Rightarrow & {\rm unpredictive\ jet/event\ structure} \end{array}$
- no easy match to hadronization
- PS : Parton Showers
 - approximate, to LL (or NLL)
 - main topology not predetermined
 - + process-generic \Rightarrow 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 $d\hat{\sigma}/dp_{\perp}^2 \approx 1/p_{\perp}^4$ for $p_{\perp} \rightarrow 0$.



MultiParton Interactions - 1

Hadrons are composite \Rightarrow many partons can interact:



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

$$\frac{\mathrm{d}\hat{\sigma}}{\mathrm{d}p_{\perp}^2} \propto \frac{\alpha_{\mathrm{s}}^2(p_{\perp}^2)}{p_{\perp}^4} \rightarrow \frac{\alpha_{\mathrm{s}}^2(p_{\perp 0}^2 + p_{\perp}^2)}{(p_{\perp 0}^2 + p_{\perp}^2)^2}$$

with $p_{\perp 0} \approx 2\text{--}3 \text{ GeV} \simeq 1/d$.

Semiperturbative 2 \rightarrow 2 generates whole nondiffractive σ ?

p

Hadrons are extended, so dependence on impact parameter b.

Overlap of protons during encounter is

$$\mathcal{O}(b) = \int \mathrm{d}^3 \mathbf{x} \, \mathrm{d}t \, \rho_1(\mathbf{x}, t) \, \rho_2(\mathbf{x}, t)$$

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

Average activity at *b* proportional to $\mathcal{O}(b)$: \star central collisions more active $\Rightarrow \mathcal{P}_n$ broader than Poissonian; \star peripheral passages normally give no collisions \Rightarrow finite $\sigma_{\text{tot.}}$.

At LHC $\langle n_{
m MPI}
angle pprox$ 3 for all events, but \gtrsim 10 for central collisions.

 $\langle n \rangle$

Jet pedestal effect – 1

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.

Jet pedestal effect -2



Double Parton Scattering



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

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



Colour Reconnection in e⁺e⁻ annihilation



At LEP 2 search for effects in $e^+e^- \rightarrow W^+W^- \rightarrow q_1\overline{q}_2 q_3\overline{q}_4$:

- perturbative $\langle \delta M_{\rm W} \rangle \lesssim 5$ MeV : negligible!
- nonperturbative $\langle \delta M_{\rm W} \rangle \sim 40 \,\,{\rm MeV}$:

favoured; no-effect option ruled out at 99.5% CL.

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

• Bose-Einstein $\langle \delta M_W \rangle \lesssim 100 \text{ MeV}$: full effect ruled out (while models with $\sim 20 \text{ MeV}$ barely acceptable).

MPIs in PYTHIA

- MPIs are gererated in a falling sequence of p⊥ values; recall Sudakov factor approach to parton showers.
- Core process QCD 2 \rightarrow 2, but also onia, γ '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. $p_{\perp 0} = p_{\perp 0}(E_{\rm cm})$, 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 ⇒ tightly packed partons ⇒ 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:

$$\begin{array}{ll} \frac{\mathrm{d}\mathcal{P}}{\mathrm{d}\boldsymbol{p}_{\perp}} & = & \left(\frac{\mathrm{d}\mathcal{P}_{\mathrm{MPI}}}{\mathrm{d}\boldsymbol{p}_{\perp}} + \sum \frac{\mathrm{d}\mathcal{P}_{\mathrm{ISR}}}{\mathrm{d}\boldsymbol{p}_{\perp}} + \sum \frac{\mathrm{d}\mathcal{P}_{\mathrm{FSR}}}{\mathrm{d}\boldsymbol{p}_{\perp}}\right) \\ & \times & \exp\left(-\int_{\boldsymbol{p}_{\perp}}^{\boldsymbol{p}_{\perp}\max} \left(\frac{\mathrm{d}\mathcal{P}_{\mathrm{MPI}}}{\mathrm{d}\boldsymbol{p}_{\perp}'} + \sum \frac{\mathrm{d}\mathcal{P}_{\mathrm{ISR}}}{\mathrm{d}\boldsymbol{p}_{\perp}'} + \sum \frac{\mathrm{d}\mathcal{P}_{\mathrm{FSR}}}{\mathrm{d}\boldsymbol{p}_{\perp}'}\right) \mathrm{d}\boldsymbol{p}_{\perp}'\right) \end{array}$$

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
- $\bullet\,$ Possible to choose two hard interactions, e.g. W^-W^-

MPI in Herwig - 1



MPI in Herwig - 2

- 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*_{⊥min} scale to be tuned energy-by-energy.
- Colour reconnection essential to get dn/dη correct.



The QCD string



QCD field lines compressed to tubelike region \Rightarrow **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.

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

$$\left|\frac{\mathrm{d}E}{\mathrm{d}z}\right| = \left|\frac{\mathrm{d}p_z}{\mathrm{d}z}\right| = \left|\frac{\mathrm{d}E}{\mathrm{d}t}\right| = \left|\frac{\mathrm{d}p_z}{\mathrm{d}t}\right| = \kappa$$

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



The Lund Model

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

Motion of quarks and antiquarks with intermediate string pieces:



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, $\tau^2 = t^2 - z^2 \sim {\rm constant},$

with breaks separated by hadronic area $m_{\perp}^2 = m^2 + p_{\perp}^2$.

Hadrons at outskirts are more boosted.

Approximately flat rapidity distribution, $dn/dy \approx constant$

 \Rightarrow total hadron multiplicity in a jet grows like ln $E_{\rm jet}$.

How does the string break?



String breaking modelled by tunneling:

$$\mathcal{P} \propto \exp\left(-rac{\pi m_{\perp q}^2}{\kappa}
ight) = \exp\left(-rac{\pi p_{\perp q}^2}{\kappa}
ight) \, \exp\left(-rac{\pi m_{q}^2}{\kappa}
ight)$$

- Common Gaussian p_{\perp} spectrum, $\langle p_{\perp} \rangle \approx 0.4$ GeV.
- Suppression of heavy quarks, $u\overline{u}: d\overline{d}: s\overline{s}: c\overline{c} \approx 1: 1: 0.3: 10^{-11}.$

• 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-Gordans needed.
- Quadratic diquark mass dependence
 - \Rightarrow strong suppression of multistrange and spin 3/2 baryons.
 - \Rightarrow effective parameters with less strangeness suppression.

The Lund gluon picture



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!

Colour flow in hard processes

One Feynman graph can correspond to several possible colour flows, e.g. for $qg \rightarrow qg$:



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



Interference terms with indeterminate colour flow $\propto 1/N_C^2$.

The Herwig cluster model



- Force $g \to q\overline{q}$ branchings.
- Porm colour singlet clusters.
- Oecay high-mass clusters to smaller clusters.
- Decay clusters to 2 hadrons according to phase space times spin weight.
 - New: allow three aligned $q\overline{q}$ clusters to reconnect to two clusters $q_1q_2q_3$ and $\overline{q}_1\overline{q}_2\overline{q}_3$.
- New: allow nonperturbative $g \rightarrow s\overline{s}$ in addition to $g \rightarrow u\overline{u}$ and $g \rightarrow d\overline{d}$.

Herwig cluster model improvement



Gieseke, Kirchgaeßer, Plätzer, EPJ C78 (2018) 99

String vs. Cluster

B^0 F^+ B^- F^+ B^- F^+ F^+ F^+ F^+ F^+ F^+ F^+ F^+ F^+ F^+ F^+ F^-		
program	PYTHIA	Herwig
model	string	cluster
energy-momentum picture	powerful	simple
	predictive	unpredictive
parameters	few	many
flavour composition	messy	simple
	unpredictive	in-between
parameters	many	few

Total cross section



DL/SaS, MBR, ABMST, RPP2016.

Diffraction

Ingelman-Schlein: Pomeron as hadron with partonic content Diffractive event = (Pomeron flux) \times (Pp collision)



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

Multiplicity in diffractive events



PYTHIA 6 lacks MPI, ISR, FSR in diffraction, so undershoots.

Spacetime evolution

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 $E_{\rm CM}/2\kappa \approx 6000$ 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!
- https://www.montecarlonet.org/

Nodes: Manchester Durham Glasgow Göttingen Karlsruhe UC London Louvain Lund

CERN Heidelberg Monash (Au) Vienna

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.

