LU TP 99–42
hep-ph/0001032
December 1999

Recent Progress in PYTHIA[1]

Torbjörn Sjöstrand[2]

Department of Theoretical Physics,
Lund University, Lund, Sweden

Abstract

PYTHIA is a general-purpose event generator for multiparticle production in high-energy physics. After a general introduction and program news survey, some areas of recent physics progress are considered: the matching to matrix elements, especially for W/Z production; charm and bottom hadronization; multiple interactions; and interconnection effects. The report concludes with some words on the future, specifically the ongoing transition to C++.

---

[1]To appear in the Proceedings of the QCD and Weak Boson Physics workshop in preparation for Run II at the Fermilab Tevatron

[2]torbjorn@thep.lu.se

1 Introduction

A general-purpose generator in high-energy physics should address a number of physics aspects, such as:

- the matrix elements for a multitude of hard subprocesses of interest,
- the convolution with parton distributions to obtain the hard-scattering kinematics and cross sections,
- resonance decays that (more or less) form part of the hard subprocess (such as W, Z, t or h),
- initial- and final-state QCD and QED showers (or, as an alternative, higher-order matrix elements, including a consistent treatment of virtual-correction terms),
- multiple parton–parton interactions,
- beam remnants,
- hadronization,
- decay chains of unstable particles, and
- general utility and analysis routines (such as jet finding).

Furthermore, one must be prepared for unexpected or less conventional effects, that could modify the assumed behaviour: the strong-interaction dynamics in QCD remains unsolved and thereby unpredictable in an absolute sense.

The PYTHIA 6.1 program was released in March 1997, as a merger of JETSET 7.4, PYTHIA 5.7 [1] and SPYTHIA [2]. It covers all of the above areas. The current subversion is PYTHIA 6.136, which contains over 50,000 lines of Fortran 77 code. The code, manuals and sample main programs may be found at
`http://www.thep.lu.se/~torbjorn/Pythia.html` .

The two other programs of a similar scope are HERWIG [3]
`http://hepwww.rl.ac.uk/theory/seymour/herwig/`
and ISAJET [4]
`ftp://penguin.phy.bnl.gov/pub/isajet` .
For parton-level processes, many more programs have been written. The availability of several generators provides for useful cross-checks and a healthy competition. Since the physics of a complete hadronic event is very complex and only partially understood from first principles, one should not prematurely converge on one single approach.

2 PYTHIA 6.1 Main News

Relative to previous versions, main news in PYTHIA 6.1 include

- a renaming of the old JETSET program elements to begin with `PY`, therefore now standard throughout,
- new SUSY processes and improved SUSY simulation relative to SPYTHIA, and new PDG codes for sparticles,
- new processes for Higgs (including doubly-charged in left–right symmetric models), technicolor, . . . ,
- several improved resonance decays, including an alternative Higgs mass shape,
- some newer parton distributions, such as CTEQ5 [5]
- initial-state showers matched to some matrix elements,
- new options for final-state gluon splitting to a pair of c/b quarks and modified

modelling of initial-state flavour excitation,

- an energy-dependent $p_{\perp\min}$ in multiple interactions,
- an improved modelling of the hadronization of small-mass strings, of importance especially for c/b, and
- a built-in package for one-dimensional histograms (based on GBOOK).

Some of these topics will be further studied below. Other improvements, of less relevance for $\overline{p}p$ colliders, include

- improved modelling of gluon emission off c/b quarks in e^+e^-,
- colour rearrangement options for W^+W^- events,
- a Bose-Einstein algorithm expanded with new options,
- a new alternative baryon production scheme [6],
- QED radiation off an incoming muon,
- a new machinery to handle real and virtual photon fluxes, cross sections and parton distributions [7], and
- new standard interfaces for the matching to external generators of two, four and six fermions (and of two quarks plus two gluons) in e^+e^-.

The current list of over 200 different subprocesses covers topics such as hard and soft QCD, heavy flavours, DIS and $\gamma\gamma$, electroweak production of γ^*/Z^0 and $W^\pm$ (singly or in pairs), production of a light or a heavy Standard Model Higgs, or of various Higgs states in supersymmetric (SUSY) or left–right symmetric models, SUSY particle production (sfermions, gauginos, etc.), technicolor, new gauge bosons, compositeness, and leptoquarks.

Needless to say, most users will still find that their particular area of interest is not as well addressed as could be wished. In some areas, progress will require new ideas, while lack of time is the limiting factor in others.

3 Matching to Matrix Elements

The matrix-element (ME) and parton-shower (PS) approaches to higher-order QCD corrections both have their advantages and disadvantages. The former offers a systematic expansion in orders of α_s, and a powerful machinery to handle multiparton configurations on the Born level, but loop calculations are tough and lead to messy cancellations at small resolution scales. Resummed matrix elements may circumvent the latter problem for specific quantities, but then do not provide exclusive accompanying events. Parton showers are based on an improved leading-log (almost next-to-leading-log) approximation, and so cannot be accurate for well separated partons, but they offer a simple, process-independent machinery that gives a smooth blending of event classes (by Sudakov form factors) and a natural match to hadronization. It is therefore natural to try to combine these descriptions, so that ME results are recovered for widely separated partons while the PS sets the subjet structure.

For final-state showers in $Z^0 \to q\overline{q}$, such solutions are the standard since long [8], e.g. by letting the shower slightly overpopulate the $q\overline{q}g$ phase space and then using a Monte Carlo veto technique to reduce down to the ME level. This approach easily carries over to showers in other colour-singlet resonance decays, although the various relevant ME's have not all been implemented in PYTHIA so far.

A similar technique is now available for the description of initial-state radiation in the production of a single colour-singlet resonance, such as $\gamma^*/Z^0/W^\pm$ [9]. The basic idea is to map the kinematics between the PS and ME descriptions, and to find a correction factor that can be applied to hard emissions in the shower so as to bring agreement with the matrix-element expression. Some simple algebra shows that, with the PYTHIA shower kinematics definitions, the two $q\overline{q}' \to gW^\pm$ emission rates disagree by a factor

$$R_{q\overline{q}'\to gW}(\hat{s},\hat{t}) = \frac{(\mathrm{d}\hat{\sigma}/\mathrm{d}\hat{t})_{\mathrm{ME}}}{(\mathrm{d}\hat{\sigma}/\mathrm{d}\hat{t})_{\mathrm{PS}}} = \frac{\hat{t}^2 + \hat{u}^2 + 2m_W^2\hat{s}}{\hat{s}^2 + m_W^4} ,$$

which is always between 1/2 and 1. The shower can therefore be improved in two ways, relative to the old description. Firstly, the maximum virtuality of emissions is raised from $Q^2_{\mathrm{max}} \approx m_W^2$ to $Q^2_{\mathrm{max}} = s$, i.e. the shower is allowed to populate the full phase space. Secondly, the emission rate for the final (which normally also is the hardest) $q \to qg$ emission on each side is corrected by the factor $R(\hat{s},\hat{t})$ above, so as to bring agreement with the matrix-element rate in the hard-emission region. In the backwards evolution shower algorithm [10], this is the first branching considered.

The other possible $\mathcal{O}(\alpha_s)$ graph is $qg \to q'W^\pm$, where the corresponding correction factor is

$$R_{qg\to q'W}(\hat{s},\hat{t}) = \frac{(\mathrm{d}\hat{\sigma}/\mathrm{d}\hat{t})_{\mathrm{ME}}}{(\mathrm{d}\hat{\sigma}/\mathrm{d}\hat{t})_{\mathrm{PS}}} = \frac{\hat{s}^2 + \hat{u}^2 + 2m_W^2\hat{t}}{(\hat{s} - m_W^2)^2 + m_W^4} ,$$

which lies between 1 and 3. A probable reason for the lower shower rate here is that the shower does not explicitly simulate the s-channel graph $qg \to q^* \to q'W$. The $g \to q\overline{q}$ branching therefore has to be preweighted by a factor of 3 in the shower, but otherwise the method works the same as above. Obviously, the shower will mix the two alternative branchings, and the correction factor for a final branching is based on the current type.

The reweighting procedure prompts some other changes in the shower. In particular, $\hat{u} < 0$ translates into a constraint on the phase space of allowed branchings.

Our published comparisons with data on the W $p_\perp$ spectrum show quite a good agreement with this improved simulation [9]. A worry was that an unexpectedly large primordial $k_\perp$, around 4 GeV, was required to match the data in the low-$p_{\perp W}$ region. However, at that time we had not realized that the data were not fully unsmeared. The required primordial $k_\perp$ is therefore likely to drop by about a factor of two [11].

It should be noted that also other approaches to the same problem have been studied recently. The HERWIG one requires separate treatments in the hard- and soft-emission regions [12]. Another, more advanced PYTHIA-based one [13], also addresses the next-to-leading order corrections to the total W cross section, while the one outlined above is entirely based on the leading-order total cross section. There is also the possibility of an extension to Higgs production [14], which is rather less trivial since already the leading-order cross section $gg \to H$ contains a QCD loop.

Summarizing, we now start to believe we can handle initial- and final-state showers, with next-to-leading-order accuracy, in cases where these can be separated by the production of colour singlet resonances — even if it should be realized that much work remains to cover the various possible cases. That still does not address the big class of QCD processes where the initial- and final-state radiation does not factorize. Possibly, correction factors to showers could be found also here. Alternatively, it may become necessary to start showers from given parton configurations of varying multiplicity and with virtual-correction weights, as obtained from higher-order ME calculations. So far, PYTHIA only implements a way to start from a given four-parton topology in e^+e^- annihilation, picking one of the possible preceding shower histories as a way to set constraints for the subsequent shower evolution [15]. This approach obviously needs to be extended in the future, to allow arbitrary parton configurations. Even more delicate will be the consistent treatment of virtual corrections [16], where much work remains.

4 Charm and Bottom Hadronization

Significant asymmetries are observed between the production of D and $\overline{D}$ mesons in $\pi^- p$ collisions, with hadrons that share some of the π^- flavour content very much favoured at large x_F in the π^- fragmentation region [17]. This behaviour was qualitatively predicted by PYTHIA; in fact, the predictions were for somewhat larger effects than seen in the data. The new data has allowed us to go back and take a critical look at the uncertainties that riddle the heavy-flavour description [18]. Many effects are involved, and we here constrain ourselves to only mentioning one.

A hadronic event is conventionally subdivided into sets of partons that form separate colour singlets. These sets are represented by strings, that e.g. stretch from a quark end via a number of intermediate gluons to an antiquark end. Three string mass regions may be distinguished for the hadronization.

1. *Normal string fragmentation.* In the ideal situation, each string has a large invariant mass. Then the standard iterative fragmentation scheme [19] works well. In practice, this approach can be used for all strings above some cut-off mass of a few GeV.
2. *Cluster decay.* If a string is produced with a small invariant mass, maybe only two-body final states are kinematically accessible. The traditional iterative Lund scheme is then not applicable. We call such a low-mass string a cluster, and consider it separately from above. In recent program versions, the modelling has now been improved to give a smooth match on to the standard string scheme in the high-cluster-mass limit.
3. *Cluster collapse.* This is the extreme case of the above situation, where the string mass is so small that the cluster cannot decay into two hadrons. It is then assumed to collapse directly into a single hadron, which inherits the flavour content of the string endpoints. The original continuum of string/cluster masses is replaced by a discrete set of hadron masses. Energy and momentum then cannot be conserved inside the cluster, but must be exchanged with the local neighbourhood of the cluster. This description has also been improved.

In general, flavour asymmetries are predicted to be smaller for bottom than for charm, and smaller at higher energies (except possibly at very large rapidities). One can therefore not expect any spectacular manifestations at the Tevatron. However, other nontrivial features do not die out as fast, like a non-negligible systematic shift between the rapidity of a heavy quark and that of the hadron produced from it [18]. The possibility of such effects should be considered whenever trying to extract any physics from heavy flavours.

5 Multiple Interactions

Multiple parton–parton interactions is the concept that, based on the composite nature of hadrons, several parton pairs may interact in a typical hadron–hadron collision [20]. Over the years, evidence for this mechanism has accumulated, such as the recent direct observation by CDF [21]. The occurences with two parton pairs at reasonably large $p_\perp$

just form the top of the iceberg, however. In the PYTHIA model, most interactions are at lower $p_\perp$, where they are not visible as separate jets but only contribute to the underlying event structure. As such, they are at the origin of a number of key features, like the broad multiplicity distributions, the significant forward–backward multiplicity correlations, and the pedestal effect under jets.

Since the perturbative jet cross section is divergent for $p_\perp \to 0$, it is necessary to regularize it, e.g. by a cut-off at some $p_{\perp\mathrm{min}}$ scale. That such a regularization should occur is clear from the fact that the incoming hadrons are colour singlets — unlike the coloured partons assumed in the divergent perturbative calculations — and that therefore the colour charges should screen each other in the $p_\perp \to 0$ limit. Also other damping mechanisms are possible [22]. Fits to data typically give $p_{\perp\mathrm{min}} \approx 2$ GeV, which then should be interpreted as the inverse of some colour screening length in the hadron.

One key question is the energy-dependence of $p_{\perp\mathrm{min}}$; this may be relevant e.g. for comparisons of jet rates at different Tevatron energies, and even more for any extrapolation to LHC energies. The problem actually is more pressing now than at the time of our original study [20], since nowadays parton distributions are known to be rising more steeply at small x than the flat $xf(x)$ behaviour normally assumed for small Q^2 before HERA. This translates into a more dramatic energy dependence of the multiple-interactions rate for a fixed $p_{\perp\mathrm{min}}$.

The larger number of partons also should increase the amount of screening, however, as confirmed by toy simulations [23]. As a simple first approximation, $p_{\perp\mathrm{min}}$ is assumed to increase in the same way as the total cross section, i.e. with some power $\epsilon \approx 0.08$ [24] that, via reggeon phenomenology, should relate to the behaviour of parton distributions at small x and Q^2. Thus the new default in PYTHIA is

$$p_{\perp\mathrm{min}} = (1.9\ \mathrm{GeV}) \left(\frac{s}{1\ \mathrm{TeV}^2} \right)^{0.08} .$$

6 Interconnection Effects

The widths of the W, Z and t are all of the order of 2 GeV. A Standard Model Higgs with a mass above 200 GeV, as well as many supersymmetric and other Beyond the Standard Model particles would also have widths in the multi-GeV range. Not far from threshold, the typical decay times $\tau = 1/\Gamma \approx 0.1\,\mathrm{fm} \ll \tau_{\mathrm{had}} \approx 1\,\mathrm{fm}$. Thus hadronic decay systems overlap, between a resonance and the underlying event, or between pairs of resonances, so that the final state may not contain independent resonance decays.

So far, studies have mainly been performed in the context of W pair production at LEP2. Pragmatically, one may here distinguish three main eras for such interconnection:

1. Perturbative: this is suppressed for gluon energies $\omega > \Gamma$ by propagator/timescale effects; thus only soft gluons may contribute appreciably.
2. Nonperturbative in the hadroformation process: normally modelled by a colour rearrangement between the partons produced in the two resonance decays and in the subsequent parton showers.
3. Nonperturbative in the purely hadronic phase: best exemplified by Bose–Einstein effects.

The above topics are deeply related to the unsolved problems of strong interactions: confinement dynamics, $1/N_{\mathrm{C}}^2$ effects, quantum mechanical interferences, etc. Thus they offer an opportunity to study the dynamics of unstable particles, and new ways to probe confinement dynamics in space and time [25, 26], *but* they also risk to limit or even spoil precision measurements.

A key gauge is the interconnection impact on W mass measurements at LEP2. Perturbative effects are not likely to give any significant contribution to the systematic error, $\langle \delta m_W \rangle \lesssim 5$ MeV [26]. Colour rearrangement is not understood from first principles, but many models have been proposed to model effects [26, 27, 28], and a conservative estimate gives $\langle \delta m_W \rangle \lesssim 40$ MeV. For Bose–Einstein again there is a wide spread in models, and an even wider one in results, with about the same potential systematic error as above [29, 30, 28]. The total QCD interconnection error is thus below m_π in absolute terms and 0.1% in relative ones, a small number that becomes of interest only because we aim for high accuracy.

A study of $e^+e^- \to t\bar{t} \to bW^+\bar{b}W^- \to b\bar{b}\ell^+\nu_\ell\ell'^-\overline{\nu}'_\ell$ near threshold gave a realistic interconnection uncertainty of the top mass of around 30 MeV, but also showed that slight mistreatments of the combined colour and showering structure could blow up this error by a factor of ten [31]. For hadronic top decys, errors could be much larger.

The above numbers, when applied to hadronic physics, are maybe not big enough to cause an immediate alarm. The addition of a coloured underlying event — with a poorly-understood multiple-interaction structure as outlined above — has not at all been considered so far, however, and can only make matters worse in hadronic physics than in e^+e^-. This is clearly a topic for the future, where we should be appropriately humble about our current understanding, at least when it comes to performing precision measurements.

QCD interconnection may also be at the root of a number of other, more spectacular effects, such as rapidity gaps and the whole Pomeron concept [32], and the unexpectedly large rate of quarkonium production [33].

7 The Future: On To C++

Finally, a word about the future. PYTHIA continues to be developed. On the physics side, there is a need to increase the support given to different physics scenarios, new and old, and many areas of the general QCD machinery for parton showers, underlying events and hadronization require further improvements, as we have seen.

On the technical side, the main challenge is a transition from Fortran to C++, the language of choice for Run II (and LHC). To address this, the PYTHIA 7 project was started in January 1998, with L. Lönnblad as main responsible. A similar project, but more ambitious and better funded, is now starting up for HERWIG, with two dedicated postdoc-level positions and a three-year time frame.

For PYTHIA, what exists today is a strategy document [34], and code for the event record, the particle object, some particle data and other data base handling, and the event generation handler structure. All of this is completely new relative to the Fortran version, and is intended to allow for a much more general and flexible formulation of the event generation process. The first piece of physics, the string fragmentation scheme, is being implemented by M. Bertini, and is nearing completion. The subprocess generation method is being worked on for the simple case of $e^+e^- \to Z^0 \to q\overline{q}$. The hope is to have a "proof of concept" version soon, and some of the current PYTHIA functionality up and running by the end of 2000. It will, however, take much further effort after that to provide a program that is both more and better than the current PYTHIA 6 version. It is therefore unclear whether PYTHIA 7 will be of much use during Run II, except as a valuable exercise for the future.

References

[1] T. Sjöstrand, Computer Phys. Commun. 82 (1994) 74.

[2] S. Mrenna, Computer Phys. Commun. 101 (1997) 232.

[3] G. Marchesini, B.R. Webber, G. Abbiendi, I.G. Knowles, M.H. Seymour and L. Stanco, Computer Phys. Commun. 67 (1992) 465.

[4] F.E. Paige, S.D. Protopopescu, H. Baer and X. Tata, hep-ph/9810440.

[5] CTEQ Collaboration, H.L. Lai et al., hep-ph/9903282.

[6] P. Edén and G. Gustafson, Z. Phys. C75 (1997) 41.

[7] C. Friberg and T. Sjöstrand, LU TP 99–11 and hep-ph/9907245, to appear in Eur. Phys. J. C.

[8] M. Bengtsson and T. Sjöstrand, Phys. Lett. B185 (1987) 435;
G. Gustafson and U. Pettersson, Nucl. Phys. B306 (1988) 746;
M.H. Seymour, Computer Phys. Commun. 90 (1995) 95.

[9] G. Miu and T. Sjöstrand, Phys. Lett. B449 (1999) 313.

[10] T. Sjöstrand, Phys. Lett. 157B (1985) 321.

[11] J Huston, these proceedings.

[12] G. Corcella and M.H. Seymour, RAL-TR-1999-051 and hep-ph/9908388.

[13] S. Mrenna, UCD-99-4 and hep-ph/9902471.

[14] S. Mrenna, in preparation.

[15] J. André and T. Sjöstrand, Phys. Rev. D57 (1998) 5767.

[16] C. Friberg and T. Sjöstrand, in 'Monte Carlo Generators for HERA Physics', eds. A.T. Doyle, G. Grindhammer, G. Ingelman and H. Jung, DESY-PROC-1999-02, p. 181.

[17] WA82 Collaboration, M. Adamovich et al., Phys. Lett. B305 (1993) 402;
E769 Collaboration, G.A. Alves et al., Phys. Rev. Lett. 72 (1994) 812;
E791 Collaboration, E.M. Aitala et al., Phys. Lett. B371 (1996) 157.

[18] E. Norrbin and T. Sjöstrand, Phys. Lett. B442 (1998) 407, in preparation.

[19] B. Andersson, G. Gustafson, G. Ingelman and T. Sjöstrand, Phys. Rep. 97 (1983) 31;
T. Sjöstrand, Nucl. Phys. B248 (1984) 469.

[20] T. Sjöstrand and M. van Zijl, Phys. Rev. D36 (1987) 2019.

[21] CDF ollaboration, F. Abe et al., Phys. Rev. Lett. 79 (1997) 584.

[22] G. Gustafson and G. Miu, LU TP 99–43.

[23] J. Dischler and T. Sjöstrand, in preparation.

[24] A. Donnachie and P.V. Landshoff, Phys. Lett. B296 (1992) 227.

[25] G. Gustafson, U. Pettersson and P. Zerwas, Phys. Lett. B209 (1988) 90.

[26] T. Sjöstrand and V.A. Khoze, Z. Phys. C62 (1994) 281, Phys. Rev. Lett. 72 (1994) 28.

[27] G. Gustafson and J. Häkkinen, Z. Phys. C64 (1994) 659;
L. Lönnblad, Z. Phys. C70 (1996) 107;
Š. Todorova–Nová, DELPHI Internal Note 96-158 PHYS 651;
J. Ellis and K. Geiger, Phys. Rev. D54 (1996) 1967, Phys. Lett. B404 (1997) 230;
B.R. Webber, J. Phys. G24 (1998) 287.

[28] J. Häkkinen and M. Ringnér, Eur. Phys. J. C5 (1998) 275.

[29] L. Lönnblad and T. Sjöstrand, Phys. Lett. B351 (1995) 293, Eur. Phys. J. C2 (1998) 165.

[30] S. Jadach and K. Zalewski, Acta Phys. Pol. B28 (1997) 1363;
V. Kartvelishvili, R. Kvatadze and R. Møller, Phys. Lett. B408 (1997) 331;
K. Fiałkowski and R. Wit, Acta Phys. Pol. B28 (1997) 2039, Eur. Phys. J. C2 (1998) 691;
Š. Todorova–Nová and J. Rameš, hep-ph/9710280.

[31] V.A. Khoze and T. Sjöstrand, Phys. Lett. B328 (1994) 466.

[32] A. Edin, G. Ingelman and J. Rathsman, Z. Phys. C75 (1997) 57

[33] A. Edin, G. Ingelman and J. Rathsman, Phys.Rev. D56 (1997) 7317

[34] L. Lönnblad, Computer Phys. Commun. 118 (1999) 213.