Chapter 1

Quarkonia sector in PYTHIA 6.2

Preliminary remarks

According to the philosophy of PYTHIA 6.2 we implemented only charmonia production processes. Nonetheless we also laid all necessary foundations to investigate the corresponding bottomonia production channels. How to run them is explained in Sect. 1.3. [**Note: This strategy implies that it is impossible to produce charmonia and bottomonia in the same run. It is not even possible to generate J/ψ and ψ' simultaneously!**]

1.1 General procedure

1.1.1 New channels

Originally only the contribution from the Colour Singlet Model (CSM) to the quarkonia production was implemented in PYTHIA 6.2. Non-relativistic Quantum Chromodynamics (NRQCD) predicts large contributions via the so-called colour octet mechanism. Therefore we introduced the following new subprocesses:

ISUB	$g+g \to c\bar{c}[n]+g$	ISUB	$q+g \to q+c\bar{c}[n]$	ISUB	$q+\bar{q} \to q+c\bar{c}[n]$
401	$g+g \to c\bar{c}[^3S_1^{(1)}]+g$				
402	$g+g \to c\bar{c}[^3S_1^{(8)}]+g$	405	$q+g \to q+c\bar{c}[^3S_1^{(8)}]$	408	$q+\bar{q} \to g+c\bar{c}[^3S_1^{(8)}]$
403	$g+g \to c\bar{c}[^1S_0^{(8)}]+g$	406	$q+g \to q+c\bar{c}[^1S_0^{(8)}]$	409	$q+\bar{q} \to g+c\bar{c}[^1S_0^{(8)}]$
404	$g+g \to c\bar{c}[^3P_J^{(8)}]+g$	407	$q+g \to q+c\bar{c}[^3P_J^{(8)}]$	410	$q+\bar{q} \to g+c\bar{c}[^3P_J^{(8)}]$

The colour singlet contribution ISUB = 401 is completely equivalent to the subprocess ISUB = 86 apart from the fact that the colour singlet model factors out the wave function $|R(0)|^2$ at the origin while NRQCD parameterizes the non-perturbative part with so-called NRQCD matrix elements. Thus, for the sake of consistency we rearranged some constants between ISUB = 86 and ISUB = 401.

In the χ_c sector there were implemented only the gluon-gluon fusion modes. We copied these modes from ISUB = 87-89 to ISUB = 411-413 rearranging some constants according to the procedure for ISUB = 86. Furthermore we provide the production mechanisms via gluon-quark and quark-antiquark fusion:

ISUB	$g+g\to c\bar{c}[^3P_J^{(1)}]+g$	ISUB	$q+g\to q+c\bar{c}[^3P_J^{(1)}]$	ISUB	$q+\bar{q}\to q+c\bar{c}[^3P_J^{(1)}]$
411	$g+g\to c\bar{c}[^3P_0^{(1)}]+g$	414	$q+g\to q+c\bar{c}[^3P_0^{(1)}]$	417	$q+\bar{q}\to q+c\bar{c}[^3P_0^{(1)}]$
412	$g+g\to c\bar{c}[^3P_1^{(1)}]+g$	415	$q+g\to q+c\bar{c}[^3P_1^{(1)}]$	418	$q+\bar{q}\to g+c\bar{c}[^3P_1^{(1)}]$
413	$g+g\to c\bar{c}[^3P_2^{(1)}]+g$	416	$q+g\to q+c\bar{c}[^3P_2^{(1)}]$	419	$q+\bar{q}\to g+c\bar{c}[^3P_2^{(1)}]$

Finally some photoproduction channels were implemented. [**Note: The tests of the proper implementation of these channels only include the expressions of the partonic amplitudes squared (i.e., the subroutine PYSIGH). One should verify at least the correct programming of the colour flow, since it was necessary to invent a configuration not used so far.**] Again the channel ISUB = 420 is equivalent to ISUB = 106 up to constants originating from the differences between NRQCD and CSM factorization:

ISUB	$g+\gamma\to c\bar{c}[^{2S+1}L_J^{(C)}]+g$	ISUB	$q+\gamma\to q+c\bar{c}[^{2S+1}L_J^{(C)}]$
420	$g+\gamma\to c\bar{c}[^3S_1^{(1)}]+g$		
421	$g+\gamma\to c\bar{c}[^3S_1^{(8)}]+g$	424	$q+\gamma\to q+c\bar{c}[^3S_1^{(8)}]$
422	$g+\gamma\to c\bar{c}[^1S_0^{(8)}]+g$	425	$q+\gamma\to q+c\bar{c}[^1S_0^{(8)}]$
423	$g+\gamma\to c\bar{c}[^3P_J^{(8)}]+g$	426	$q+\gamma\to q+c\bar{c}[^3P_J^{(8)}]$

1.1.2 New parameters - the NRQCD matrix elements

Analogously to the Colour Singlet Model NRQCD parameterizes the non-perturbative fragmentation of the $Q\overline{Q}$ pair into the quarkonium state. However, the extension on colour octet modes demands additional parameters. While the CSM goes with only two parameters, the wave function at the origin squared $|R(0)|^2$ (PARP(38)) and its derivative $|R'(0)|^2$ (PARP(39)), NRQCD needs five independent matrix elements $\langle\mathcal{O}^H[^{2S+1}L_J^{(C)}]\rangle$ to denote the probability that a $Q\overline{Q}$ pair in the quantum state $^{2S+1}L_J^{(C)}$ build up the bound state H:

$$\texttt{PARP(195)}: \quad \langle\mathcal{O}^{J/\psi}[{}^3S_1^{(1)}]\rangle \tag{1.1a}$$

$$\texttt{PARP(196)}: \quad \langle\mathcal{O}^{J/\psi}[{}^3S_1^{(8)}]\rangle \tag{1.1b}$$

$$\texttt{PARP(197)}: \quad \langle\mathcal{O}^{J/\psi}[{}^1S_0^{(8)}]\rangle \tag{1.1c}$$

$$\texttt{PARP(198)}: \quad \frac{\langle\mathcal{O}^{J/\psi}[{}^3P_0^{(8)}]\rangle}{m_c^2} \tag{1.1d}$$

$$\texttt{PARP(199)}: \quad \frac{\langle\mathcal{O}^{\chi_{c0}}[{}^3P_0^{(1)}]\rangle}{m_c^2} \tag{1.1e}$$

Their default values are set to one. [**This should be changed later!**] The relation between the colour singlet matrix element and the wave function at the origin is given by

$$\langle\mathcal{O}^{J/\psi}[{}^3S_1^{(1)}]\rangle = \frac{3N_c}{2\pi}|R(0)|^2\,, \tag{1.2a}$$

$$\langle\mathcal{O}^{\chi_{c0}}[{}^3P_0^{(1)}]\rangle = \frac{3N_c}{2\pi}|R'(0)|^2\,. \tag{1.2b}$$

Moreover, the matrix elements fulfill the following relations due to heavy quark spin symmetry:

$$\langle\mathcal{O}^{J/\psi}[{}^3P_J^{(8)}]\rangle = (2J+1)\langle\mathcal{O}^{J/\psi}[{}^3P_0^{(8)}]\rangle\,, \tag{1.3a}$$

$$\langle\mathcal{O}^{\chi_{cJ}}[{}^3P_J^{(1)}]\rangle = (2J+1)\langle\mathcal{O}^{\chi_{c0}}[{}^3P_0^{(1)}]\rangle\,. \tag{1.3b}$$

1.1.3 New states and their fragmentation

Since the colour octet $c\bar{c}$ pair were not known by PYTHIA 6.2 we had to define new "particles". We used the convention, that the `KF` code for a colour octet states is obtained by adding 70000 to the `KF` code for the corresponding colour singlet state. The new particles are:

$$\begin{array}{ll} \texttt{KF}(c\bar{c}[{}^3S_1^{(8)}]) = 70443 & \texttt{KF}(b\bar{b}[{}^3S_1^{(8)}]) = 70553 \\ \texttt{KF}(c\bar{c}[{}^1S_0^{(8)}]) = 70441 & \texttt{KF}(b\bar{b}[{}^1S_0^{(8)}]) = 70551 \\ \texttt{KF}(c\bar{c}[{}^3P_0^{(8)}]) = 80441 & \texttt{KF}(b\bar{b}[{}^3P_0^{(8)}]) = 80551 \end{array} \tag{1.4}$$

In order to respect the possible phase space restrictions the fragmentation of the $Q\overline{Q}$ pair into the quarkonium H is described as decay process. Hence, e.g., the large colour octet contributions seen in the J/ψ energy spectrum from HERA for $z \to 1$ should be naturally suppressed since in the colour octet channels there is no phase space left to radiate of (a) soft gluon(s). PYTHIA now knows the following decay channels:

$$\begin{array}{llll} \texttt{IDC} = \texttt{4500}: & c\bar{c}[^3S_1^{(8)}] \to J/\psi + g & \texttt{IDC} = \texttt{4503}: & b\bar{b}[^3S_1^{(8)}] \to \Upsilon + g \\ \texttt{IDC} = \texttt{4501}: & c\bar{c}[^1S_0^{(8)}] \to J/\psi + g & \texttt{IDC} = \texttt{4504}: & b\bar{b}[^1S_0^{(8)}] \to \Upsilon + g \\ \texttt{IDC} = \texttt{4502}: & c\bar{c}[^3P_0^{(8)}] \to J/\psi + g & \texttt{IDC} = \texttt{4505}: & b\bar{b}[^3P_0^{(8)}] \to \Upsilon + g \end{array} \qquad (1.5)$$

The branching ratio for these decays is one and the decay width of the colour octet $Q\overline{Q}$ pairs is set to 0.1 GeV by default. We choose their masses to be about 30 MeV larger than the one of the quarkonium bound state, which is some lower bound set by PYTHIA. [**Note: NRQCD requires two soft gluons for the transition of a $^3S_1$ octet state into the corresponding quarkonium. Therefore one could think about adding a second gluon in the final state of decay channels `4500` and `4503` as well as enhancing the mass of the $Q\overline{Q}$ pair with respect to the other colour octet channels.**]

1.1.4 Remarks on masses

PYTHIA needs the colour octet $Q\overline{Q}$ pair to be heavier (by about 30 MeV) than the corresponding bound state to allow for the decay processes in (1.5). Within the framework the mass difference between the $Q\overline{Q}$ pair and the bound state is predicted to be of the order

$$M_{Q\overline{Q}} - M_H \sim m_Q v^2 \qquad (1.6)$$

where v is the typical non-relativistic velocity of the heavy (anti)quarks inside the quarkonium H.

Our value is considerably smaller which takes into account the fact that the NRQCD matrix elements usually are fitted with a mass value of $m_c = 1.5(5)$ GeV and $m_b = 4.8(8)$, respectively. Since on the one hand the partonic amplitude squared is quite sensitive on the heavy quark mass while its exact value is only known up to orders of $m_Q v^2$ (see 1.6) it is difficult to give any strict prescription for the mass handling. [**In PYTHIA it should even be possible to randomize the mass of the $Q\overline{Q}$ pair, e.g. within a Gaussian of the width $m_Q v^2$ and a value $m_Q v^2$ above the mass of the bound state.**]

1.1.5 Altarelli-Parisi evolution

The contribution $Q\overline{Q}[^3S_1^{(8)}]$ partly comes from the fragmentation of a gluon. Since this gluon could have splitted into two gluons before the fragmentation we have to provide a possibility for mimicking this effect. We invented two new switches, namely `MSTJ(191)` to switch on and of the splitting

$$Q\overline{Q}[^3S_1^{(8)}] \to Q\overline{Q}[^3S_1^{(8)}] + g \qquad (1.7)$$

and MSTJ(192) to choose if it is ensured that the $Q\overline{Q}$ pair always takes the larger fraction of the four-momentum. [**Still I am not completely convinced that these switch works properly!**] The evolution (1.7) obeys the Altarelli-Parisi evolution for $g \to g + g$.

Since the fragmentation contribution of $Q\overline{Q}[^3S_1^{(8)}]$ production processes is the more important the higher the transverse momentum of the $Q\overline{Q}$ pair is it is advisable to switch on the Altarelli-Parisi evolution for events with large transverse momentum.

[**One could think about deciding to switch on the Altarelli-Parisi evolution on an event-by-event basis in the same way how it is decided which colour flow has to be taken.**]

1.1.6 Polarization

We also implemented the hard partonic amplitude squared splitted into its density matrix elements $\rho_{\lambda_1,\lambda_2}$. Thus the polarized cross sections are available as long as on does not insist on the proper angular distribution for the muons from the quarkonium decay. Their distribution in PYTHIA is always assumed to be spherical though this is not even true for "unpolarized" production if we assume that the quarkonia polarization is dependent on the transverse momentum of the quarkonium. The variable MSTP(195) allows to switch from unpolarized generation of quarkonia (MSTP(195) = 0) to the generation of distinct helicity states (or distinct components of the density matrix element):

$$\texttt{MSTP(195)} = \texttt{1} \tag{1.8}$$

We took the expressions for the density matrix elements from [1] and [2] for J/ψ and χ production, respectively. In the former paper the result is given for several frames. In general one is free to choose the frame in which the polarization should be calculated. The values of MSTP(196) refer to several reference frames: recoil frame (= 1), Gottfried Jackson frame (= 2), target frame (= 3), and Collins Soper frame (= 4). For definitions of these frame see [1]. However, since the standard PYTHIA output provides all particle energies and momenta in the recoil frame all distributions of an helicity state or a density matrix element component are only available in the recoil frame, too. Therefore we highly recommend to use only

$$\texttt{MSTP(196)} = \texttt{1} \tag{1.9}$$

To get distributions in other frames, it is necessary to rotate and boost the particle four-momenta first [**which probably could be realized using the PYTHIA subroutine PYROBO**].

The helicity state (or the component of the density matrix element $\rho_{\lambda_1,\lambda_2}$) is selected by the value of the switch MSTP(197). For values ≤ 2 MSTP(197) denotes the modulus of the $Q\overline{Q}$ pair helicity λ (cf. [2])

$$\texttt{MSTP(197)} = |\lambda| \tag{1.10}$$

while `MSTP(197) = 3`, `MSTP(197) = 4`, `MSTP(197) = 5`, and `MSTP(197) = 6` correspond to the components $\rho_{0,0}$, $\rho_{1,1}$, $\rho_{1,0}$, and $\rho_{1,-1}$ of the density matrix element, respectively (cf. [1]).

1.2 Explicit changes

We have changed four subroutines in the PYTHIA 6.2 code:

- PYDATA: set all necessary parameters
- PYSCAT: set colour flow and kinematics
- PYSIGH: provide partonic amplitudes squared
- PYSHOW: enable Altarelli-Parisi evolution

NOTE: All the changes are embedded into:

```
C...QUARKONIA+++
...
C...QUARKONIA---
```

1.2.1 The subroutine PYDATA

In this subroutine all the information about the particle content of the subprocesses, the properties of these particles ... is given:

Subprocesses:

To define the provided subprocesses the following sets of variables is used:

`ISUB`	number of the subprocess
`PROC(ISUB)`	name of subprocess `ISUB`
`KFPR(ISUB,1), KFPR(ISUB,2)`	KF flavour code of products in subprocess `ISUB`
`ISET(ISUB)`	switch for subprocess `ISUB`

In order to avoid mistakes we tried to copy as much information as possible from other subprocesses. Promising candidates for being templates should have similar particle content. Thus not only the J/ψ (`ISUB = 86`) and χ (`ISUB = 87-89`) production modes served as source we also lend information from the Higgs production processes $q + g \to q + h_0$ (`ISUB = 112`) and $q + \bar{q} \to g + h_0$ (`ISUB = 111`).

ISUB	PROC(ISUB)	KFPR(ISUB,... 1)	2)	ISET(ISUB)
401	g + g -> QQ~[3S11] + g	443	21	2
402	g + g -> QQ~[3S18] + g	70443	21	2
403	g + g -> QQ~[1S08] + g	70441	21	2
404	g + g -> QQ~[3PJ8] + g	80441	21	2
405	q + g -> q + QQ~[3S18]	0	70443	2
406	q + g -> q + QQ~[1S08]	0	70441	2
407	q + g -> q + QQ~[3PJ8]	0	80441	2
408	q + q~ -> g + QQ~[3S18]	21	70443	2
409	q + q~ -> g + QQ~[1S08]	21	70441	2
410	q + q~ -> g + QQ~[3PJ8]	21	80441	2
411	g + g -> QQ~[3P01] + g	10441	21	2
412	g + g -> QQ~[3P11] + g	20443	21	2
413	g + g -> QQ~[3P21] + g	445	21	2
414	q + g -> q + QQ~[3P01]	0	10441	2
415	q + g -> q + QQ~[3P11]	0	20443	2
416	q + g -> q + QQ~[3P21]	0	445	2
417	q + q~ -> g + QQ~[3P01]	21	10441	2
418	q + q~ -> g + QQ~[3P11]	21	20443	2
419	q + q~ -> g + QQ~[3P21]	21	445	2
420	g + gamma -> QQ~[3S11] + g	443	21	2
421	g + gamma -> QQ~[3S18] + g	70443	21	2
422	g + gamma -> QQ~[1S08] + g	70441	21	2
423	g + gamma -> QQ~[3PJ8] + g	80441	21	2
424	q + gamma -> q + QQ~[3S18]	0	70443	2
425	q + gamma -> q + QQ~[1S08]	0	70441	2
426	q + gamma -> q + QQ~[3PJ8]	0	80441	2

The "strange" order of the particles is determined by the pattern of the source processes. Note also that we only generate ${}^3P_0^{(8)}$ states (`KFPR(ISUB,.) = 80441`!) in the P wave production processes `ISUB = 404, 407, 410, 423, 426`. In fact the states ${}^3P_1^{(8)}$ and ${}^3P_2^{(8)}$ are implicitly incorporated (cf. eq. (1.3a)).

Particle properties:

As mentioned above we had to include the colour octet $Q\overline{Q}$ states as new particles. We chose some `KC` away from other particles to ensure compatibility with forthcoming versions of PYTHIA. The following parameters fix the properties of particles inside PYTHIA:

`KC`	compressed particle code
`CHAF(KC)`	particle name
`KCHG(KC,1|2|3|4)`	3 times charge — colour — own antiparticle — KF code
`PMAS(KC,1|2|3|4)`	mass — width — mass deviation — lifetime
`MDCY(KC,1|2|3)`	decay allowed — decay channel — number of decay modes
`MWID(KC)`	character of particle width

		KCHG(KC,...				PMAS(KC,...				MDCY(KC,...			
KC	CHAF(KC)	1)	2)	3)	4)	1)	2)	3)	4)	1)	2)	3)	MWID(KC)
450	cc~[3S18]	0	2	0	70443	3.1	0.01	0	0	1	4500	1	2
451	cc~[1S08]	0	2	0	70441	3.1	0.01	0	0	1	4501	1	2
452	cc~[3P08]	0	2	0	80441	3.1	0.01	0	0	1	4502	1	2
453	bb~[3S18]	0	2	0	70553	9.5	0.01	0	0	1	4503	1	2
454	bb~[1S08]	0	2	0	70551	9.5	0.01	0	0	1	4504	1	2
455	bb~[3P08]	0	2	0	80551	9.5	0.01	0	0	1	4505	1	2

Particle decay properties:

We also tried to keep the numbers `IDC` of the decay channels away form other decay modes even though it seems to be difficult to ensure compatibility with forthcoming PYTHIA versions. The properties of the particle decays are defined by:

`IDC`	number of decay channel
`MDME(IDC,1|2)`	switch for channel `IDC` — special treatment of matrix element
`BRAT(IDC)`	branching ration of channel `IDC`
`KFDP(IDC,1|2|3|4|5)`	decay products 1–5 of channel `IDC`

IDC	MDME(IDC,... 1)	2)	BRAT(IDC)	KFDP(IDC,... 1)	2)	3)	4)	5)
4500	1	51	1	443	21	0	0	0
4501	1	51	1	443	21	0	0	0
4502	1	51	1	443	21	0	0	0
4503	1	51	1	553	21	0	0	0
4504	1	51	1	553	21	0	0	0
4505	1	51	1	553	21	0	0	0

NRQCD matrix elements:

The values for NRQCD matrix elements are denoted by the parameters `PARP(195)` - `PARP(199)`:

$\langle \mathcal{O}^{J/\psi}[^{(2S+1)}L_J^{(C)}]\rangle$	I	PARP(I)
$\langle \mathcal{O}^{J/\psi}[^3S_1^{(1)}]\rangle$	195	1.
$\langle \mathcal{O}^{J/\psi}[^3S_1^{(8)}]\rangle$	196	1.
$\langle \mathcal{O}^{J/\psi}[^1S_0^{(8)}]\rangle$	197	1.
$\langle \mathcal{O}^{J/\psi}[^3P_0^{(8)}]\rangle/m_c^2$	198	1.
$\langle \mathcal{O}^{\chi_{c0}}[^3P_0^{(1)}]\rangle/m_c^2$	199	1.

Altarelli-Parisi evolution:

The handling of the Altarelli-Parisi evolution of the $Q\overline{Q}[^3S_1^{(8)}]$ state is done with the help of the switches `MSTJ(191)` (Default = 0) and `MSTJ(192)` (Default = 0):

`MSTJ(191) = 0`: Altarelli-Parisi evolution for $Q\overline{Q}[^3S_1^{(8)}]$ switched off
`MSTJ(191) = 1`: Altarelli-Parisi evolution for $Q\overline{Q}[^3S_1^{(8)}]$ switched on

`MSTJ(192) = 0`: daughter $Q\overline{Q}[^3S_1^{(8)}]$ picks always the larger momentum fraction ($z \geq 0.5$)
`MSTJ(192) = 1`: daughter $Q\overline{Q}[^3S_1^{(8)}]$ picks momentum fraction randomly ($\langle z\rangle = 0.5$)

Polarization:

The polarization state of the generated charmonia we control via the switch `MSTP(195)`, `MSTP(196)`, and `MSTP(197)`. While the first parameter tells if the unpolarized cross section is calculated or just on helicity component

`MSTP(195) = 0`: unpolarized partonic amplitude squared
`MSTP(195) = 1`: density matrix element (chosen by `MSTP(197)`)

the remaining switches serves to choose the reference frame and the helicity state (or the component of the density matrix element $\rho_{\lambda_1,\lambda_2}$):

`MSTP(196)`	frame
1	recoil
2	Gottfried Jackson
3	target
4	Collins Soper

`MSTP(197)`	$\vert\lambda\vert$	$\rho_{\lambda_1,\lambda_2}$
0	0	
1	1	
2	2	
3		$\rho_{0,0}$
4		$\rho_{1,1}$
5		$\rho_{1,0}$
6		$\rho_{1,-1}$

1.2.2 The subroutine `PYSCAT`

This subroutine sets kinematics and the colour flow of the partonic process. The changes we made are mainly copied from other subprocesses:

Kinematics:

$$\text{For}\left\{\begin{array}{c} g+g\to Q\overline{Q}+g \\ q+g\to q+Q\overline{Q} \\ q+\bar{q}\to g+Q\overline{Q} \\ g+\gamma\to Q\overline{Q}+g \\ q+\gamma\to q+Q\overline{Q} \end{array}\right\} \begin{array}{c}\texttt{MINT(21)}\text{ and }\texttt{MINT(22)} \\ \text{are ``copied'' from}\end{array} \left\{\begin{array}{c} g+g\to J/\psi,\chi_{cJ}+g \\ q+g\to q+h_0 \\ q+\bar{q}\to g+h_0 \\ g+\gamma\to J/\psi,\chi_{cJ}+g \\ q+\gamma\to q+Z \end{array}\right.$$

`MINT(21)` and `MINT(22)` are the flavour codes KF for the outgoing partons from the hard interaction.

Colour flow:

$$\text{For}\left\{\begin{array}{c} g+g\to Q\overline{Q}[^3S_1^{(1)}]+g \\ g+g\to Q\overline{Q}[^{(2S+1)}L_J^{(8)}]+g \\ q+g\to q+Q\overline{Q}[^{(2S+1)}L_J^{(8)}] \\ q+\bar{q}\to g+Q\overline{Q}[^{(2S+1)}L_J^{(8)}] \\ g+\gamma\to Q\overline{Q}[^3S_1^{(1)}]+g \\ g+\gamma\to Q\overline{Q}[^{(2S+1)}L_J^{(8)}]+g \\ q+\gamma\to q+Q\overline{Q}[^{(2S+1)}L_J^{(8)}] \end{array}\right\}\begin{array}{c}\texttt{KCC}\text{ (and }\texttt{KCS}\text{)}\\ \text{are copied from}\end{array}\left\{\begin{array}{c} g+g\to J/\psi,\chi_{cJ}+g \\ g+g\to g+g \\ q+g\to q+g \\ q+\bar{q}\to g+g \\ g+\gamma\to J/\psi+g \\ \text{no correspondence !} \\ q+\gamma\to q+g \end{array}\right.$$

KCC and KCS are internal variables to define the colour structure of the hard interaction.

	MINT(21), MINT(22) from ...	KCC, KCS from ...
ISUB = 401	ISUB = 86-89	ISUB = 86-89
402 ≤ ISUB ≤ 404	ISUB = 86-89	ISUB = 68
405 ≤ ISUB ≤ 407	ISUB = 112	ISUB = 28
408 ≤ ISUB ≤ 410	ISUB = 111	ISUB = 13
411 ≤ ISUB ≤ 413	ISUB = 86-89	ISUB = 86-89
414 ≤ ISUB ≤ 416	ISUB = 112	ISUB = 112
417 ≤ ISUB ≤ 419	ISUB = 111	ISUB = 111
ISUB = 420	ISUB = 107	ISUB = 107
421 ≤ ISUB ≤ 423	ISUB = 107	?!
424 ≤ ISUB ≤ 426	ISUB = 35	ISUB = 33

1.2.3 The subroutine PYSIGH

This subroutine contains the partonic amplitude squared (up to an factor $1/(16\pi^2)$). At this stage we also multiply with the NRQCD matrix element to ensure a proper relative weighting if several channels are run at the same time.

New quarkonia production channels and NRQCD matrix elements:

ISUB	production channel
401	$g + g \to c\bar{c}[^3S_1^{(1)}] + g$
402	$g + g \to c\bar{c}[^3S_1^{(8)}] + g$
403	$g + g \to c\bar{c}[^1S_0^{(8)}] + g$
404	$g + g \to c\bar{c}[^3P_J^{(8)}] + g$
405	$q + g \to q + c\bar{c}[^3S_1^{(8)}]$
406	$q + g \to q + c\bar{c}[^1S_0^{(8)}]$
407	$q + g \to q + c\bar{c}[^3P_J^{(8)}]$
408	$q + \bar{q} \to g + c\bar{c}[^3S_1^{(8)}]$
409	$q + \bar{q} \to g + c\bar{c}[^1S_0^{(8)}]$
410	$q + \bar{q} \to g + c\bar{c}[^3P_J^{(8)}]$

ISUB	production channel
411	$g + g \to c\bar{c}[^3P_0^{(1)}] + g$
412	$g + g \to c\bar{c}[^3P_1^{(1)}] + g$
413	$g + g \to c\bar{c}[^3P_2^{(1)}] + g$
414	$q + g \to q + c\bar{c}[^3P_0^{(1)}]$
415	$q + g \to q + c\bar{c}[^3P_1^{(1)}]$
416	$q + g \to q + c\bar{c}[^3P_2^{(1)}]$
417	$q + \bar{q} \to g + c\bar{c}[^3P_0^{(1)}]$
418	$q + \bar{q} \to g + c\bar{c}[^3P_1^{(1)}]$
419	$q + \bar{q} \to g + c\bar{c}[^3P_2^{(1)}]$

ISUB	production channel
420	$g + \gamma \to c\bar{c}[^3S_1^{(1)}] + g$
421	$g + \gamma \to c\bar{c}[^3S_1^{(8)}] + g$
422	$g + \gamma \to c\bar{c}[^1S_0^{(8)}] + g$
424	$g + \gamma \to c\bar{c}[^3P_J^{(8)}] + g$
424	$q + \gamma \to q + c\bar{c}[^3S_1^{(8)}]$
425	$q + \gamma \to q + c\bar{c}[^1S_0^{(8)}]$
426	$q + \gamma \to q + c\bar{c}[^3P_J^{(8)}]$

PARP(I)	$\langle \mathcal{O}^{J/\psi}[^{(2S+1)}L_J^{(C)}]\rangle$
PARP(195)	$\langle \mathcal{O}^{J/\psi}[^3S_1^{(1)}]\rangle$
PARP(196)	$\langle \mathcal{O}^{J/\psi}[^3S_1^{(8)}]\rangle$
PARP(197)	$\langle \mathcal{O}^{J/\psi}[^1S_0^{(8)}]\rangle$
PARP(198)	$\langle \mathcal{O}^{J/\psi}[^3P_0^{(8)}]\rangle/m_c^2$
PARP(199)	$\langle \mathcal{O}^{\chi_{c0}}[^3P_0^{(1)}]\rangle/m_c^2$

It is necessary to be careful with the Mandelstam variables `TH` and `UH` since they are interchanged with respect to [1] and [2] for $408 \leq$ `ISUB` ≤ 410 and $417 \leq$ `ISUB` ≤ 424. Also one should be conscious of the parton number of the quark-antiquark pair, i.e., $401 \leq$ `ISUB` ≤ 404 and $411 \leq$ `ISUB` ≤ 413 the squared mass of the $Q\overline{Q}$ pair is given by `SQM3` while in the other subprocesses holds `SQMQQ = SQM4`.

Polarization:

The polarization state is controlled by `MSTP(195) - MSTP(197)`:

MSTP(195)	$\|\mathcal{A}\|^2$
0	unpolarized
1	polarized

MSTP(196)	frame
1	recoil
2	Gottfried Jackson
3	target
4	Collins Soper

MSTP(197)	$\|\lambda\|$	$\rho_{\lambda_1,\lambda_2}$
0	0	
1	1	
2	2	
3		$\rho_{0,0}$
4		$\rho_{1,1}$
5		$\rho_{1,0}$
6		$\rho_{1,-1}$

Colour flow:

The colour flow trough the hard partonic subprocess is important to obtain a proper fragmentation picture of a process since the fragmentation is highly correlated with colour strings stemming from the perturbative kernel. In the partonic calculation we can define the colour flow only on the basis of Feynman diagrams, i.e., each Feynman diagram allow for a special set of colour flow configurations. For the process $g+g \to g+g$ for example, there are three diagrams (s, t, and u channel exchange) for each of them there are two allowed colour configurations. In this case PYTHIA calculates the amplitude squared of each diagram and weights the corresponding colour configurations accordingly. The problem is that the amplitude squared also contains interaction terms between two Feynman diagrams. There it is impossible to assign a definite colour configuration. However, the problem is not too bad since:

$$|\mathcal{A}_1 + \mathcal{A}_2 + \mathcal{A}_3|^2 = |\mathcal{A}_1|^2 + |\mathcal{A}_2|^2 + |\mathcal{A}_3|^2 + \mathcal{O}\left(\frac{1}{N_c}\right) \tag{1.11}$$

We copied the weighting for the different colour flows from the "equivalent" processes $g+g \to g+g$, $q+g \to q+g$, and $q+\bar{q} \to g+g$. This procedure is not really appropriate since it ignores the $Q\overline{Q}$ mass but proper weighting would need the partonic matrix element splitted into the different contributions stemming from different colour topologies. At least the solution so far is a first approach. Note that for the calculation of the relative weights of the colour topologies we needed to redefine the Mandelstam variables (`TH` $\to$ `THP`, `UH` $\to$ `UHP`) to respect the masslessness of the gluon in contrast to the massive colour octet $c\bar{c}$ state.

1.2.4 The subroutine `PYSHOW`

In this subroutine the showering of the partons is simulated. We implied a Altarelli-Parisi splitting for the $c\bar{c}[^3S_1^{(8)}]$ and the $b\bar{b}[^3S_1^{(8)}]$ state to mimic the gluon splitting that precedes the fragmentation process. The problem is that not all $Q\overline{Q}[^3S_1^{(8)}]$ contributions stem from fragmentation. Hence, it would be better to switch on the Altarelli-Parisi evolution selectively. However, one would need the matrix elements splitted into the different contributions again. [**A possible solution would look like this: (1) Weight (as in for the colour flow) the contribution from fragmentation and non-fragmentation diagrams. (Is there any kind of suppression for the interaction terms as the $1/N_c$ for colours??) (2) Define ratio $x = |\mathcal{A}_{\mathbf{frag}}|^2/(|\mathcal{A}_{\mathbf{frag}}|^2 + |\mathcal{A}_{\mathbf{non\text{-}frag}}|^2)$. (3) Randomize a number between zero and on an compare this number with x. If it is smaller switch on the Altarelli-Parisi evolution.**]

(Default: `= 0`)	AP evolution
`MSTJ(191) = 0`	off
`MSTJ(191) = 1`	on

It is also provided a switch that enables to decide weather the $Q\overline{Q}$ pair should always take the larger fraction of the parent four-momentum or if the four-momentum should be distributed randomly between the daughters:

(Default: `= 0`)	momentum fraction of $Q\overline{Q}[^3S_1^{(8)}]$
`MSTJ(192) = 0`	hard ($z \geq 0.5$)
`MSTJ(192) = 1`	randomly ($\langle z \rangle = 0.5$)

1.3 Bottomonia and higher states

As in the original version of PYTHIA 6.2 we only implemented subprocesses for the charmonium sector, and there, to be precise, only for the lowest angular momentum state. However, PYTHIA knows the particle properties for the corresponding bottomonia states as well. Hence, results in the bottomonia sector are available, too. Therefore you just have to change the outgoing $c\bar{c}$ states in the subprocesses $\texttt{401} \leq \texttt{ISUB} \leq \texttt{426}$ to the corresponding $b\bar{b}$ states:

$$\begin{array}{ll} \left.\begin{array}{l} \texttt{401} \leq \texttt{ISUB} \leq \texttt{404} \\ \texttt{411} \leq \texttt{ISUB} \leq \texttt{413} \end{array}\right\} & \texttt{KFPR(ISUB,1)} = \texttt{KFPR(ISUB,1)} + \texttt{110} \\ \left.\begin{array}{l} \texttt{405} \leq \texttt{ISUB} \leq \texttt{410} \\ \texttt{414} \leq \texttt{ISUB} \leq \texttt{426} \end{array}\right\} & \texttt{KFPR(ISUB,2)} = \texttt{KFPR(ISUB,2)} + \texttt{110} \end{array} \tag{1.12}$$

and to use the corresponding set of NRQCD matrix elements:

$$
\begin{aligned}
\texttt{PARP(195)}: &\quad \langle \mathcal{O}^{J/\psi}[^3S_1^{(1)}]\rangle \to \langle \mathcal{O}^{\Upsilon}[^3S_1^{(1)}]\rangle \\
\texttt{PARP(196)}: &\quad \langle \mathcal{O}^{J/\psi}[^3S_1^{(8)}]\rangle \to \langle \mathcal{O}^{\Upsilon}[^3S_1^{(8)}]\rangle \\
\texttt{PARP(197)}: &\quad \langle \mathcal{O}^{J/\psi}[^1S_0^{(8)}]\rangle \to \langle \mathcal{O}^{\Upsilon}[^1S_0^{(8)}]\rangle \\
\texttt{PARP(198)}: &\quad \langle \mathcal{O}^{J/\psi}[^3P_0^{(8)}]\rangle/m_c^2 \to \langle \mathcal{O}^{\Upsilon}[^3P_0^{(8)}]\rangle/m_b^2 \\
\texttt{PARP(199)}: &\quad \langle \mathcal{O}^{\chi_{c0}}[^3P_0^{(1)}]\rangle/m_c^2 \to \langle \mathcal{O}^{\chi_{b0}}[^3P_0^{(1)}]\rangle/m_b^2
\end{aligned}
$$

The corresponding procedure for the channels $86 \leq \texttt{ISUB} \leq 89$ is described in the PYTHIA manual.

The story for the higher states ψ' and $\Upsilon(2S)$ (Since PYTHIA 6.2 doesn't know the particle and decay properties of the $\Upsilon(3S)$ the implementation of its production processes needs more work.) is slightly more complicated. Although the colour singlet channel is easily adjusted by

$$\texttt{KFPR(401,1)} = \texttt{KFPR(401,1)} + 100000 \tag{1.13}$$

and changing the value `PARP(195)` for the NRQCD matrix element:

$$
\begin{aligned}
\langle \mathcal{O}^{J/\psi}[^3S_1^{(1)}]\rangle &\to \langle \mathcal{O}^{\psi'}[^3S_1^{(1)}]\rangle \\
\langle \mathcal{O}^{\Upsilon(1S)}[^3S_1^{(1)}]\rangle &\to \langle \mathcal{O}^{\Upsilon(2S)}[^3S_1^{(1)}]\rangle
\end{aligned} \tag{1.14}
$$

the colour states would still decay into a J/ψ and a $\Upsilon(1S)$, respectively. Therefore also the decay properties of the $c\bar{c}$ and $b\bar{b}$ pair, respectively, have to be adjusted:

$c\bar{c} \to \psi' + g$	$b\bar{b} \to \Upsilon(2S) + g$
$\texttt{KFDP(4500,1)} = \texttt{KFDP(4500,1)} + 100000$	$\texttt{KFDP(4503,1)} = \texttt{KFDP(4503,1)} + 100000$
$\texttt{KFDP(4501,1)} = \texttt{KFDP(4501,1)} + 100000$	$\texttt{KFDP(4504,1)} = \texttt{KFDP(4504,1)} + 100000$
$\texttt{KFDP(4502,1)} = \texttt{KFDP(4502,1)} + 100000$	$\texttt{KFDP(4505,1)} = \texttt{KFDP(4505,1)} + 100000$

Note that in this case the mass of the $c\bar{c}$ ($b\bar{b}$) pair has to be larger than the mass of the ψ' ($\Upsilon(2S)$), which mass on its part has to be larger than the mass of the J/ψ ($\Upsilon(1S)$). Since the partonic cross section is quite sensitive on the quark mass this could possibly cause some troubles for comparing the results with forthcoming investigations.

Bibliography

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