MBR Monte Carlo Simulation in PYTHIA8

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Abstract

We present the MBR (Minimum Bias Rockefeller) Monte Carlo simulation of (anti) proton-proton interactions and its implementation in the PYTHIA8 event generator. We discuss the total, elastic, and total-inelastic cross sections, and three contributions from diffraction dissociation processes that contribute to the latter: single diffraction, double diffraction, and central diffraction or double-Pomeron exchange. The event generation follows a renormalized-Regge-theory model, successfully tested using CDF data. Based on the MBR-enhanced PYTHIA8 simulation, we present cross-section predictions for the LHC and beyond, up to collision energies of 50 TeV.

1 Introduction

The MBR (Minimum Bias Rockefeller) Monte Carlo (MC) simulation is an event generator addressing the contributions of three diffraction-dissociation processes to the total-inelastic pp cross section[1]: single-diffraction dissociation or single dissociation (SD), in which one of the incoming protons dissociates, double-diffraction dissociation or double dissociation (DD), in which both protons dissociate, and central dissociation (CD) or double-Pomeron exchange (DPE), where neither proton dissociates. These processes are tabulated below,

$$\begin{aligned} \text{SD} \quad & pp \to Xp \\ \text{or} \quad & pp \to pY \\ \text{DD} \quad & pp \to XY \\ \text{CD (DPE)} \quad & pp \to pXp, \end{aligned}$$

where X and Y represent diffractively dissociated protons. Schematic diagrams are shown in Fig. 1, along with diagrams for the total and elastic cross sections, which are also simulated in MBR.

MBR predicts the energy dependence of the total, elastic, and total-inelastic pp cross sections, and fully simulates the above three diffractive components of the total-inelastic cross section. The diffractive-event generation is based on a phenomenological renormalized-Regge-theory model[1], originally developed for the CDF experiment. We have implemented MBR in PYTHIA8[2], where it can be activated with the flag: `Diffraction:PomFlux` = 5.

[1]Although the original MBR addresses several hadron-hadron collisions, including $\bar{p}p$, we will be assuming pp collisions throughout this paper for simplicity, except as explicitly stated.

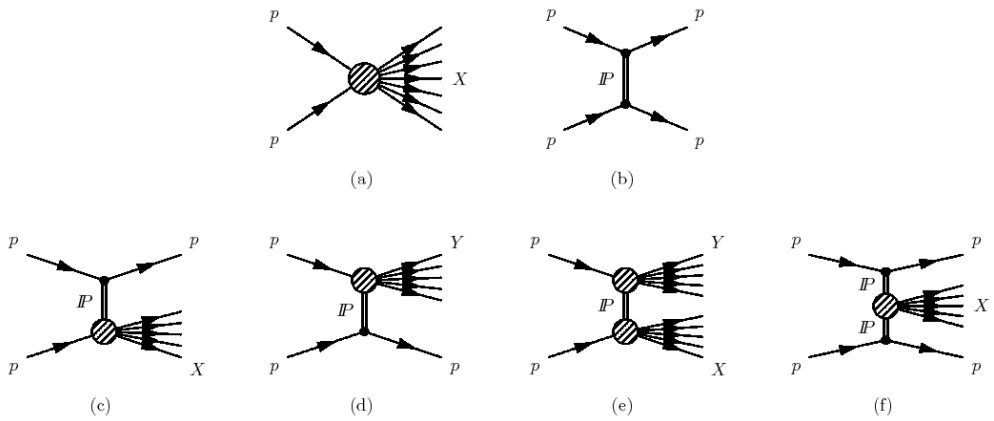


Figure 1: Schematic diagrams of soft pp processes addressed in MBR: (a) total cross section, (b) elastic scattering, (c)-(d) single diffraction or single dissociation (SD), (e) double diffraction or double dissociation (DD), and (f) central diffraction (CD) or double-Pomeron exchange (DPE).

This paper is organized as follows: in Sec. 2 we present the formulae used to calculate the total and elastic cross sections, as well as the diffractive and non-diffractive components of the total-inelastic cross section; in Sec. 3 we describe details of the generation of diffractive events; and in Sec. 4 we summarize the PYTHIA8 "steering cards" for employing MBR in the simulation.

2 Cross sections

The total cross section ($\sigma_{\rm tot}$) is the sum of the total-elastic ($\sigma_{\rm el}$) and total-inelastic ($\sigma_{\rm inel}$) cross sections. The $\sigma_{\rm tot}$ and $\sigma_{\rm el}$ are calculated in Sec. 2.1. The total-inelastic cross section ($\sigma_{\rm inel}$) is obtained as $\sigma_{\rm inel} = \sigma_{\rm tot} - \sigma_{\rm el}$. The $\sigma_{\rm inel}$ receives contributions from the diffractive components (SD, DD, CD or DPE) and from the non-diffractive (ND) cross section, defined as:

$$\sigma_{\rm ND} = (\sigma_{\rm tot} - \sigma_{\rm el}) - (2\sigma_{\rm SD} + \sigma_{\rm DD} + \sigma_{\rm CD}), \tag{1}$$

where $\sigma_{\rm SD}$ is the cross section for either $pp \to Xp$ or $pp \to pY$, assumed to be equal. The diffractive cross sections are calculated in Sec. 2.2.

2.1 Total, elastic, and total-inelastic cross sections

The $\sigma_{\rm tot}^{p^{\pm}p}(s)$ cross sections at a pp center-of-mass-energy $\sqrt{s}$ are calculated as follows:

$$\sigma_{\rm tot}^{p^{\pm}p} = \begin{cases} 16.79 s^{0.104} + 60.81 s^{-0.32} \mp 31.68 s^{-0.54} & \text{for } \sqrt{s} < 1.8 \text{ TeV}, \\ \sigma_{\rm tot}^{\rm CDF} + \frac{\pi}{s_0}\left[\left(\ln\frac{s}{s_F}\right)^2 - \left(\ln\frac{s^{\rm CDF}}{s_F}\right)^2\right] & \text{for } \sqrt{s} \geq 1.8 \text{ TeV}, \end{cases} \tag{2}$$

The term for $\sqrt{s} < 1.8$ TeV, where the $(\pm)$ denotes $\binom{p}{\bar{p}}$, is obtained from a global Regge-theory fit to pre-LHC data on $p^{\pm}p$, $K^{\pm}p$ and $\pi^{\pm}p$ cross sections [3], while that for $\sqrt{s} \geq 1.8$ TeV is a prediction of a model based on a saturated Froissart bound[4]. The latter, which

we normalize to the CDF measurement of $\sigma_{\rm tot}$ at $\sqrt{s^{\rm CDF}} = 1.8$ TeV, $\sigma_{\rm tot}^{\rm CDF} = 80.03 \pm 2.24$ mb, depends on two parameters: the energy at which the saturation occurs, $\sqrt{s_F} = 22$ GeV, and the energy-scale parameter, s_0, for which we use $s_0 = 3.7 \pm 1.5$ mb.

The elastic cross section, $\sigma_{\rm el}^{p^{\pm}p}$, is calculated using $\sigma_{\rm tot}$ from Eq. (2), multiplied by the elastic-to-total cross-section ratio, $\sigma_{\rm el}/\sigma_{\rm tot}$, obtained from the global Regge fit of Ref. [3]. The total inelastic cross section is calculated as $\sigma_{\rm inel} = \sigma_{\rm tot} - \sigma_{\rm el}$.

The energy dependences of $\sigma_{\rm tot}$, $\sigma_{\rm el}$ and $\sigma_{\rm inel}$ are shown in Fig. 2, and cross-section values at $\sqrt{s}$=0.3, 0.9, 1.96, 2.76, 7, 8 and 14 TeV are presented in Tab. 1.

2.2 Diffractive cross sections

Cross sections for SD, DD and CD (or DPE) are calculated using a phenomenological model discussed in detail in Ref. [1]. Differential cross sections are expressed in terms of the Pomeron ($I\!P$) trajectory, $\alpha(t) = 1 + \epsilon + \alpha' t = 1.104 + 0.25\ ({\rm GeV}^{-2}) \cdot t$, the Pomeron-proton coupling, $\beta(t)$, and the ratio of the triple-$I\!P$ to the $I\!P$-proton couplings, $\kappa \equiv g(t)/\beta(0)$. For sufficiently large rapidity gaps ($\Delta y \gtrsim 3$), for which $I\!P$-exchange dominates, the cross sections may be written as,

$$\frac{d^2\sigma_{SD}}{dt d\Delta y} = \frac{1}{N_{\rm gap}(s)} \left[\frac{\beta^2(t)}{16\pi} e^{2[\alpha(t)-1]\Delta y} \right] \cdot \left\{ \kappa\beta^2(0) \left(\frac{s'}{s_0} \right)^{\epsilon} \right\}, \tag{3}$$

$$\frac{d^3\sigma_{DD}}{dt d\Delta y dy_0} = \frac{1}{N_{\rm gap}(s)} \left[\frac{\kappa\beta^2(0)}{16\pi} e^{2[\alpha(t)-1]\Delta y} \right] \cdot \left\{ \kappa\beta^2(0) \left(\frac{s'}{s_0} \right)^{\epsilon} \right\}, \tag{4}$$

$$\frac{d^4\sigma_{DPE}}{dt_1 dt_2 d\Delta y dy_c} = \frac{1}{N_{\rm gap}(s)} \left[\Pi_i \left[\frac{\beta^2(t_i)}{16\pi} e^{2[\alpha(t_i)-1]\Delta y_i} \right] \right] \cdot \kappa \left\{ \kappa\beta^2(0) \left(\frac{s'}{s_0} \right)^{\epsilon} \right\}, \tag{5}$$

where t is the square of the four-momentum-transfer at the proton vertex and Δy is the rapidity gap width. The variable y_0 in Eq. (4) is the center of the rapidity gap. In Eq. (5), the subscript $i = 1, 2$ enumerates Pomerons in the DPE event, $\Delta y = \Delta y_1 + \Delta y_2$ is the total (sum of two gaps) rapidity-gap width in the event, and y_c is the center in η of the centrally-produced hadronic system.

Eqs. (3) and (4) are equivalent to those of standard-Regge theory, as ξ, the fractional forward-momentum-loss of the surviving proton (forward momentum carried by $I\!P$), is related to the rapidity gap by $\xi = e^{-\Delta y}$. The variable ξ is defined as $\xi_{\rm SD} = M^2/s$ and $\xi_{\rm DD} = M_1^2 M_2^2/(s \cdot s_0)$, where M^2 (M_1^2, M_2^2) are the masses of dissociated systems in SD (DD) events. For DD events, $y_0 = \frac{1}{2}\ln(M_2^2/M_1^2)$, and for DPE $\xi = \xi_1\xi_2 = M^2/s$.

The Pomeron-proton coupling , $\beta(t)$, is given by:

$$\beta^2(t) = \beta^2(0) F^2(t), \tag{6}$$

where $\beta(0) = 4.0728\ \sqrt{\rm mb} = 6.566\ {\rm GeV}^{-1}$ and $F(t)$ is the proton form factor from Ref. [5]:

$$F^2(t) = \left[\frac{4m_p^2 - 2.8t}{4m_p^2 - t} \left(\frac{1}{1 - \frac{t}{0.71}} \right)^2 \right]^2 \approx a_1 e^{b_1 t} + a_2 e^{b_2 t}. \tag{7}$$

The right-hand side of Eq. (7) is a double-exponential approximation of $F^2(t)$, with a_1 =0.9, a_2=0.1, b_1 =4.6 GeV^{-2}, and b_2 =0.6 GeV^{-2}. The term in curly brackets in Eqs.(3)-(5) is the $I\!P$-p total cross section at the reduced $I\!P$-p collision energy squared, $s' = s \cdot e^{-\Delta y}$. The parameter κ is set to $\kappa = 0.17$ [9], and $\kappa\beta^2(0) \equiv \sigma_0$, where σ_o defines the total Pomeron-proton cross section at an energy-squared value of $s_0 = 1$ GeV^2, is set to $\sigma_0 = 2.82$ mb or 7.249 GeV^{-2}.

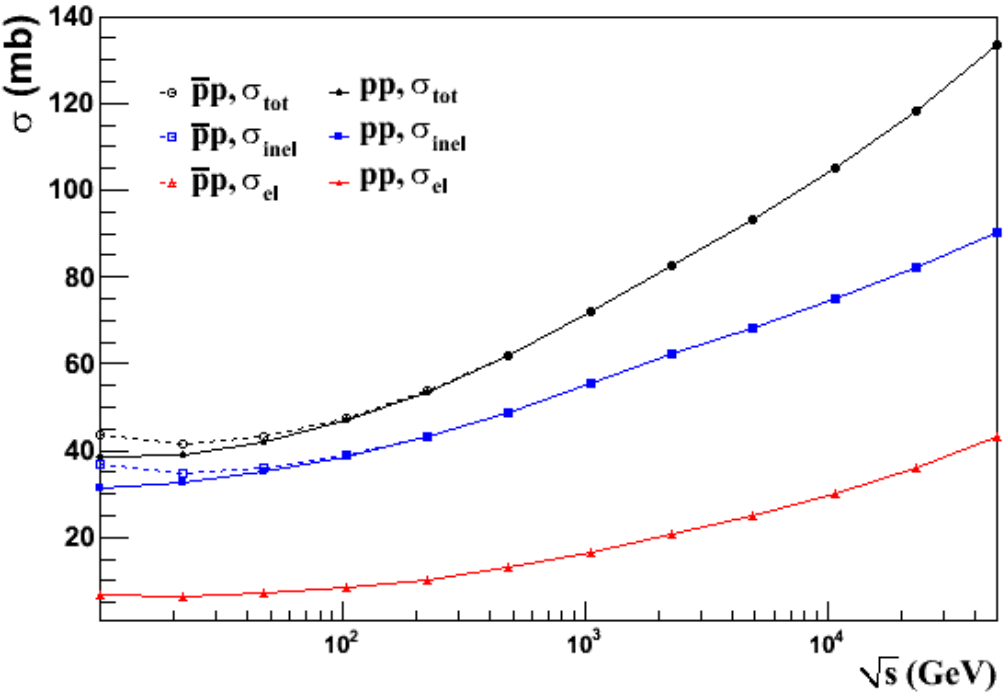


Figure 2: Total, elastic and total-inelastic pp and $\bar{p}p$ cross sections vs. $\sqrt{s}$.

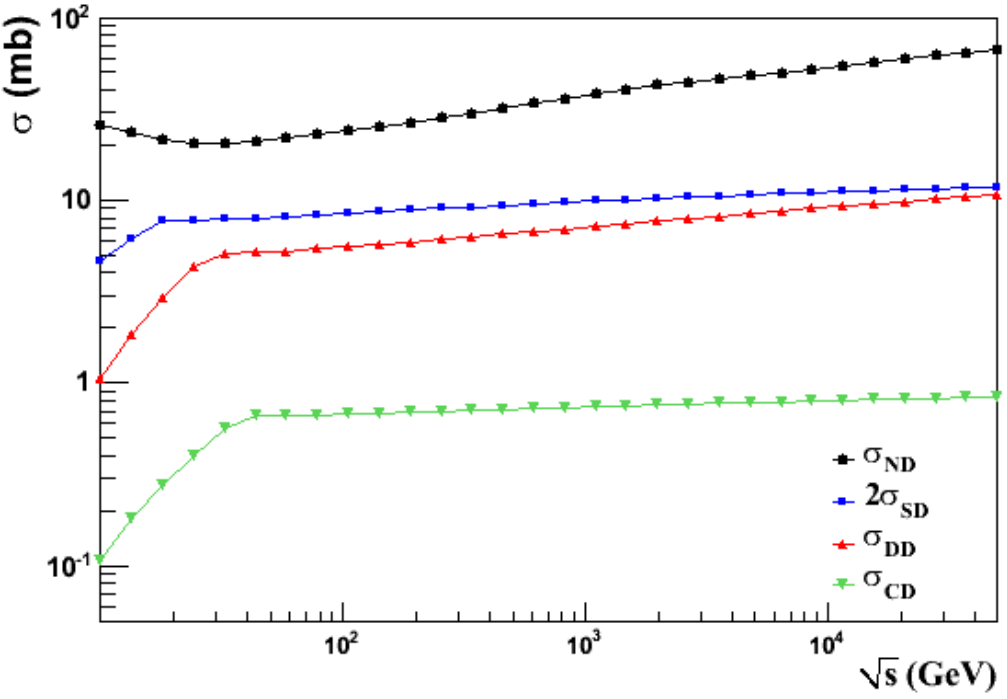


Figure 3: Diffractive (SD, DD, CD) and non-diffractive (ND) cross sections vs. $\sqrt{s}$.

$\sqrt{s}$ (TeV)	0.3	0.9	1.96	2.76	7	8	14
$\sigma_{\rm tot}$	56.50	69.87	81.03	85.25	98.29	100.35	109.49
$\sigma_{\rm el}$	11.28	15.83	19.97	21.70	27.20	28.09	32.10
$\sigma_{\rm inel}$	45.23	54.04	61.06	63.55	71.10	72.26	77.39
σ_{ND}	29.19	36.50	42.41	44.39	50.57	51.54	55.84
σ_{2SD}	9.10	9.76	10.22	10.41	10.91	10.98	11.26
σ_{DD}	6.21	7.03	7.67	7.97	8.82	8.94	9.47
σ_{CD}	0.718	0.746	0.766	0.776	0.800	0.804	0.818

Table 1: Cross sections in mb of the processes contributing to the Minimum-Bias sample, calculated as explained in Sec. 2.1 and Sec. 2.2, for selected values of $\sqrt{s}$.

Pointing again to Eqs.(3)-(5, the renormalization parameter, $N_{\rm gap}(s)$, is defined as $N_{\rm gap}(s) = min(1, f)$, where f is the integral of the term in square brackets, corresponding to a Pomeron flux. The integral is calculated over all phase space in t_i and in η_0 (DD) or η_c (DPE) for $\Delta y > 2.3$. The renormalization procedure we use, which is based on interpreting the Pomeron flux as a (diffractive) gap-formation probability, yields predictions which are in very good agreement with diffractive measurements at CDF[6, 7, 8].

The cross-section formulae are used to generate events with large (diffractive) rapidity gaps, Δy. We suppress cross sections at small value of Δy by multiplying Eqs. (3)-(5) by:

$$S = \frac{1}{2}\left[1 + erf\left(\frac{\Delta y - \Delta y_S}{\sigma_S}\right)\right], \tag{8}$$

where erf is the error function [10], centered by default at $\Delta y_S = 2$ with a width of $\sigma_S = 0.5$. For SD, this choice corresponds to suppressing events above the coherence limit ($\xi \lesssim 0.135$) [11]. For DD, the choice of $\Delta y_S = 2$ is somewhat arbitrary, because of the difficulty of unambiguously distinguishing a low-Δy DD event from a ND event with a rapidity gap from (exponentially suppressed) fluctuations. Changing Δy_S introduces event migrations between DD and ND samples. Such migrations have no impact on the total-inelastic cross section, as can be inferred from Eq. (1). For DPE, the suppression is applied to the total-gap width, $\Delta y = \Delta y_1 + \Delta y_2$.

Fig. 3 presents the energy dependence of diffractive cross sections calculated as explained above. The non-diffractive cross section, given by Eq. (1) is also shown. Cross-section values for $\sqrt{s}$=0.3, 0.9, 1.96, 2.76, 7, 8 and 14 TeV are tabulated in Tab. 1.

3 Event generation

The four-momenta of particles produced in the event are generated as described below, in Secs. 3.1-3.3. The results of the simulation for SD and DD at $\sqrt{s} = 7$ TeV are presented in Fig. 4, which shows differential cross sections as a function of rapidity-gap width, Δy, compared to predictions of PYTHIA8-4C (rescaled Schüler & Sjöstrand model[2], `Diffraction:PomFlux = 1`). The distribution of $d\sigma/d\Delta y$ vs. the total rapidity-gap-width, $\Delta y = \Delta y_1 + \Delta y_2$, and vs. the width of an individual gap, Δy_1, for CD at $\sqrt{s} = 7$ TeV is shown in Fig. 5.

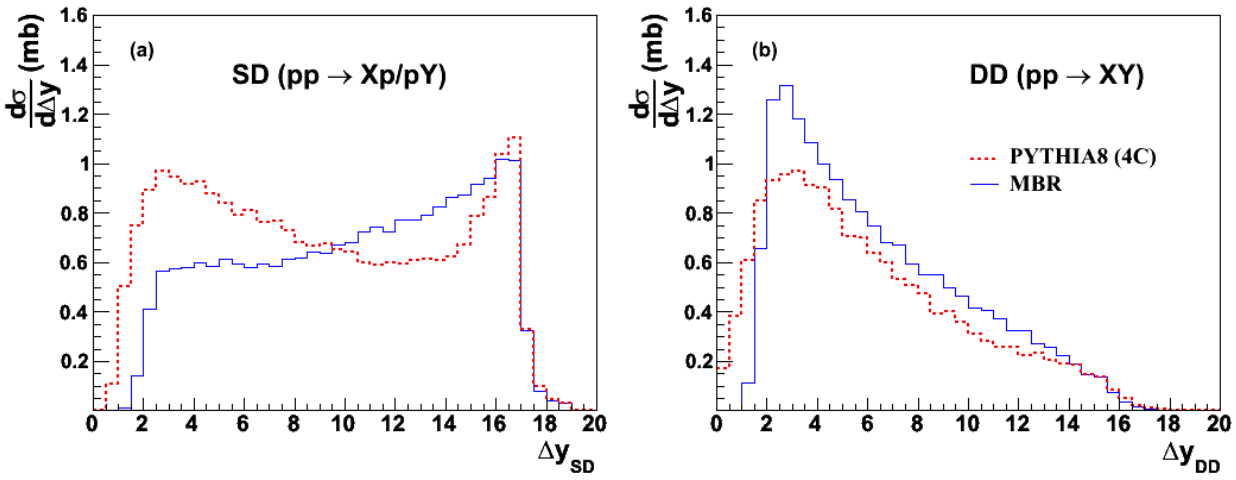


Figure 4: Differential cross sections as a function of Δy for (a) SD and (b) DD at $\sqrt{s} = 7$ TeV, compared to predictions of PYTHIA8-4C (rescaled Schüler & Sjöstrand model[2], `Diffraction:PomFlux=1`).

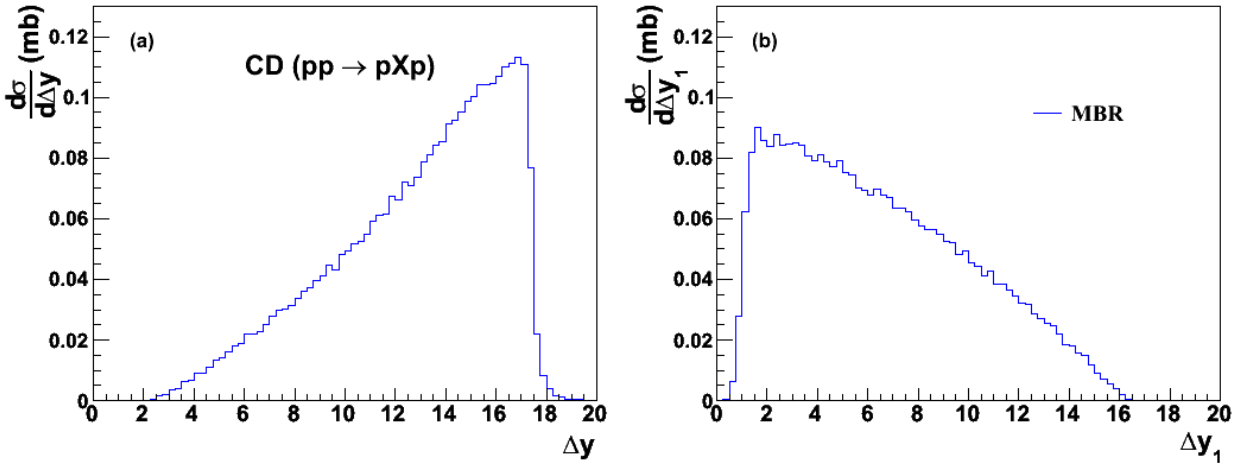


Figure 5: Differential cross sections for CD (DPE) at $\sqrt{s} = 7$ TeV as a function of: (a) total-gap width ($\Delta y = \Delta y_1 + \Delta y_2$), and (b) single-gap width (Δy_1).

3.1 Single-diffractive events

Events are generated by first choosing the rapidity-gap width, Δy, according to Eq. (3) integrated over t:

$$\frac{d\sigma_{SD}}{d\Delta y} \sim e^{\epsilon \Delta y} \cdot \left(\frac{a_1}{b_1 + 2\alpha' \Delta y} + \frac{a_2}{b_2 + 2\alpha' \Delta y} \right) \cdot S. \tag{9}$$

The range of the generation is defined by $\Delta y_{min} = 0$ and $\Delta y_{max} = -\ln M_0^2/s$, where $M_0^2 =$MBR`m2Min`. The term:

$$S = \frac{1}{2} \left[1 + erf \left(\frac{\Delta y - \text{MBR}\texttt{dyminSD}}{\text{MBR}\texttt{dyminSigSD}} \right) \right], \tag{10}$$

is added to suppress events at low values of Δy, as explained in Sec. 2.2.

A value of t is then chosen according to:

$$\frac{d\sigma_{SD}}{dt} \sim F^2(t) \cdot e^{2\alpha' \Delta y t}, \tag{11}$$

where $F^2(t)$ is given by Eq. (7) and the integration is performed up to $t_{max} = -m_p^2 \cdot \frac{\xi^2}{1-\xi}$, with $\xi = e^{-\Delta y}$. The diffractive mass is calculated as $M = \sqrt{s\xi}$. The four-momenta of the outgoing proton and the dissociated mass system are calculated using Mandelstam variables for a two-body scattering process, as implemented in PYTHIA8 for other `Diffraction:PomFlux` options.

3.2 Double-diffractive events

Events are generated by first choosing the rapidity-gap width according to Eq. (4) integrated over t. Eq. (4) is divergent as $\Delta y \to 0$. In order to remove the divergence, the integration over t is performed within the limits from $t_{min} = -e^{\Delta y}$ to $t_{max} = -e^{-\Delta y}$. Then, Δy is chosen from the distribution:

$$\frac{d\sigma_{DD}}{d\Delta y} \sim e^{\epsilon \Delta y} \cdot \frac{\ln \frac{s s_0}{M_0^4} - \Delta y}{2\alpha' \Delta y} \left(e^{-2\alpha' \Delta y e^{-\Delta y}} - e^{-2\alpha' \Delta y e^{\Delta y}} \right) \cdot S, \tag{12}$$

and the range of the generation is defined by $\Delta y_{min} = 0$ and $\Delta y_{max} = -\ln M_0^4/(s s_0)$, where $M_0^2 =$ MBR`m2Min` and $s_0 = 1$ GeV^2. To further suppress events at low values of Δy the term:

$$S = \frac{1}{2} \left[1 + erf \left(\frac{\Delta y - \text{MBR}\texttt{dyminDD}}{\text{MBR}\texttt{dyminSigDD}} \right) \right], \tag{13}$$

is used as explained in Sec. 2.2.

The variable t is chosen according to:

$$\frac{d\sigma_{DD}}{dt} \sim e^{2\alpha' \Delta y t}, \tag{14}$$

in the range from $t_{min} = -e^{\Delta y}$ to $t_{max} = -e^{-\Delta y}$.

Then, the center of the rapidity gap, y_0, is selected uniformly within the limits:

$$-\frac{1}{2} \left(\ln \frac{s s_0}{M_0^4} - \Delta y \right) < y_0 < \frac{1}{2} \left(\ln \frac{s s_0}{M_0^4} - \Delta y \right), \tag{15}$$

and the diffractive masses are calculated as:

$$M_1^2 = \sqrt{s \cdot e^{-\Delta y - y_0}}, \tag{16}$$

$$M_2^2 = \sqrt{s \cdot e^{-\Delta y + y_0}}. \tag{17}$$

The four-momenta of the outgoing dissociated mass systems are calculated using Mandelstam variables for a two-body scattering process, as implemented in PYTHIA8 for other options of `Diffraction:PomFlux` .

3.3 Central-diffractive (DPE) events

Events are generated by first choosing the total rapidity gap width, Δy, according to Eq. (5), integrated over t_1 and t_2:

$$\frac{d\sigma_{CD}}{d\Delta y} \sim e^{\epsilon\Delta y} \int_{-\Delta y/2+y_0}^{\Delta y/2-y_0} dy_0 \; f_- \cdot f_+ \cdot S_1 S_2, \tag{18}$$

where:

$$f_\pm = \left(\frac{a_1}{b_1 + \alpha'\Delta y \pm 2\alpha' y_0} + \frac{a_2}{b_2 + \alpha'\Delta y \pm 2\alpha' y_0} \right), \tag{19}$$

and the integration is performed from $\Delta y_{min} = 0$ to $\Delta y_{max} = -\ln M_0^2/s$, where $M_0^2 =$`MBRm2Min`. For events at low values of Δy we suppress individual gaps with the factor:

$$S = \frac{1}{2}\left[1 + erf\left(\frac{\Delta y - \text{MBR}\texttt{dyminCD}/2}{\text{MBR}\texttt{dyminSigCD}/\sqrt{2}}\right)\right]. \tag{20}$$

Then, the direction of the centrally-produced hadronic system, y_c, is selected uniformly within the region:

$$-\frac{1}{2}\left(\Delta y - \Delta y_{min}\right) < y_c < \frac{1}{2}\left(\Delta y - \Delta y_{min}\right), \tag{21}$$

and rapidity gaps corresponding to each of the two Pomerons are calculated as:

$$\Delta y_1 = \Delta y/2 + y_0, \tag{22}$$

$$\Delta y_2 = \Delta y/2 - y_0. \tag{23}$$

The four-momentum transfers squared at each proton vertex, t_1 and t_2, are generated according to:

$$\frac{d\sigma_{CD,i}}{dt} \sim F^2(t_i) \cdot e^{2\alpha'\Delta y_i t_i}, \tag{24}$$

up to $t_{max,i} = -m_p^2 \cdot \frac{\xi_i^2}{1-\xi_i}$, where $\xi_i = e^{-\Delta y_i}$ and $i = 1, 2$. Then, the p_T and p_z of outgoing protons are calculated as $p_{T,i}^2 = (1-\xi_i)|t_i| - m_p^2\xi_i^2$ and $|p_{z,i}| = p(1-\xi_i)$, where $p = \sqrt{s/4 - m_p^2}$ is the incoming proton momentum.

Finally, the four-momentum of the hadronic system is calculated from the sum of the four-momenta of the Pomerons, each calculated as a difference between the incoming and outgoing proton four-vectors.

4 MBR implementation in PYTHIA8

The MBR generation is activated with the following flag: `Diffraction:PomFlux = 5`. The simulation works for the pp, $p\bar{p}$ and $\bar{p}p$ scattering, and the beam setup is checked in the PYTHIA8 initialization step. It is assumed that the user will veto the event generation, after `Pythia::init() = false` is returned for other beam particles.

The simulation of the CD (DPE) process is implemented in PYTHIA8 for the first time. It is activated with the flag `SoftQCD:centralDiffractive = on`. The corresponding-process

number is set to 106, naturally extending the list of soft QCD processes[2]. In the event record, the outgoing protons' information is written in rows 3 and 4, and the centrally-dissociated hadronic system occupies row 5 (represented by the `rho_diff0` pseudo-particle).

Below, we present the default values of parameters, used when the MBR simulation is activated:

- the parameters of the Pomeron trajectory, $\alpha(t) = 1 + \epsilon + \alpha' t$:

```
Diffraction:MBRepsilon = 0.104
Diffraction:MBRalpha = 0.25
```

- the Pomeron-proton coupling, $\beta(0)$ (GeV^{-1}), and the total Pomeron-proton cross section, σ_0 (mb), see Sec. 2.2:

```
Diffraction:MBRbeta0 = 6.566
Diffraction:MBRsigma0 = 2.82
```

- the lowest mass-squared value of the dissociated system, M_0^2, used to evaluate the highest allowed rapidity gap width, Δy_{max}, see Sec. 3:

```
Diffraction:MBRm2Min = 1.5
```

- the minimum width of the rapidity gap used in the calculation of $N_{\mathrm{gap}}(s)$ (flux renormalization, Sec. 2.2):

```
Diffraction:MBRdyminSDflux = 2.3
Diffraction:MBRdyminDDflux = 2.3
Diffraction:MBRdyminCDflux = 2.3
```

- the parameters Δy_S and σ_S, used for the cross-section suppression at low Δy (non-diffractive region), see Eq. (8):

```
Diffraction:MBRdyminSD = 2.0
Diffraction:MBRdyminDD = 2.0
Diffraction:MBRdyminCD = 2.0

Diffraction:MBRdyminSigSD = 0.5
Diffraction:MBRdyminSigDD = 0.5
Diffraction:MBRdyminSigCD = 0.5
```

In addition, if the option `Diffraction:PomFlux = 5` is set, no dampening of the diffractive cross sections is performed (no effect of `SigmaDiffractive:dampen = on`); however, the user can still set his/her own cross sections by hand (`SigmaTotal:setOwn= on`).

[2] 103 and 104 for SD with proton dissociation along the positive or negative z-axis, respectively, and 105 for DD.

5 Summary

We present the MBR (Minimum Bias Rockefeller) Monte Carlo simulation, which has been tested using CDF data, and discuss its implementation in the PYTHIA8 generator. The double-Pomeron-exchange process is included in PYTHIA8 for the first time. The simulation is designed to apply to all Minimum Bias processes in the LHC energy range.

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