

1 Pythia 8.3 tuning based on Belle fragmentation related  
2 measurements

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9 **Abstract**

10 Belle has measured a large number of fragmentation-related results that  
11 have been already successfully used in global fits of fragmentation functions.  
12 These fragmentation functions are important input for studying the nucleon  
13 structure in semi-inclusive Deeply inelastic lepton nucleon scattering and  
14 hadron collisions. Apart from the additional flavor-sensitivity, also spin and  
15 transverse momentum of partons in the nucleon can be accessed this way. Ad-  
16 ditionally, these fragmentation-related results should be extremely sensitive  
17 to the fragmentation parameters in Monte Carlo event generators. This note  
18 concentrates on the tuning efforts of PYTHIA 8.3 using these measurements.

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<sup>272</sup> **1 To-Do list and Changelog**

<sup>273</sup> **1.1 README**

<sup>274</sup> **1.2 To-Do list**

<sup>275</sup> • add sensitivity discussion for popcorn variables

<sup>276</sup> **1.3 Changelog v1.0 → v2.0**

<sup>277</sup> • Added candle plot with best values in comparison to default and Belle2 values

## 278 2 Introduction

279 Fragmentation describes the formation of confined final-state hadrons from high-  
280 energetic, asymptotically free partons. Just as parton distribution functions, they  
281 cannot be calculated from first principles in QCD and therefore need to be extracted  
282 experimentally. For the same reason, also Monte Carlo event generators have to use  
283 models to describe this. One of the most commonly used models is the Lund string  
284 fragmentation model. While the Lund model can describe the fragmentation reason-  
285 ably well, overall, it relies on many parameters that need to be tuned using data.  
286 In this note this tuning was performed systematically on the various fragmentation  
287 measurements that contain sensitivities to the main Lund parameters, the suppres-  
288 sion of strange quark pairs produced in the fragmentation, the suppression of  $\eta$   
289 mesons, the suppression of di-quark pair production needed to create baryons in the  
290 fragmentation, the transverse momentum generated in the fragmentation, and the  
291 role vector mesons and higher spin particle production has over the pseudoscalar  
292 production, etc.

293 In the following the procedure to tune the fragmentation parameters are dis-  
294 cussed. Initially the different types of software and their setups are discussed. Then,  
295 the sensitivities of the used measurements to the relevant variables are discussed  
296 before the actual fit results and best tune parameters are presented and discussed.

### 297 2.1 The Lund Model

298 The Lund String fragmentation model [1, 2] is the main model that tries to describe  
299 the fragmentation process. It generally describes  $e^+e^-$  fragmentation into hadrons as  
300 the separation of singlet (anti)quarks moving away from each other within a linear  
301 potential that quasi-classically describes the QCD confining potential. The linear  
302 potential can be thought of being caused by a string of gluons connecting the two  
303 color charges. This string then eventually breaks up into a quark-antiquark pair  
304 (or also diquark-antidiquark pair). These resulting (anti-)quarks either coalesce into  
305 hadrons or expand further, creating even more quark-antiquark pairs in the process.  
306 In this stochastic process particles are then produced according to

$$f(z) = N \frac{1}{z} (1-z)^a \exp\left(-\frac{bm^2}{z}\right) \quad (1)$$

307 where  $a$  defines how fast the function vanishes at high- $z$  and  $b$  is related to the mass  
308 created at a certain  $z$ , and  $z$  is the energy fraction a hadron carries relative to the  
309 initial parton energy. Furthermore, this generation does not have to necessarily fol-  
310 low on the lightcone, but can also happen at transverse coordinates, thus allowing  
311 for transverse momentum to be generated relative to the initially separating par-  
312 tons. Empirically, not all quark-antiquark pairs can be created equally, as heavier  
313 quarks are less likely to be created in the fragmentation process. For this purpose  
314 a parameter was introduced that describes the suppression of strangeness relative  
315 to light quark flavors. The model is initially also not a priori able to distinguish  
316 between what spin-state a certain hadron that was created has. Therefore parame-  
317 ters for vector meson generation over pseudo-scalar generation for light, strange and

<sup>318</sup> charm quarks are introduced, as well as similar parameters for spin, orbital angular  
<sup>319</sup> and total angular momenta up to 2 are introduced.

### <sup>320</sup> **3 Tuning Setup, prerequisites, etc**

<sup>321</sup> For the general setup, Pythia 8.3.12 (later also 8.3.16 to be discussed below, see A)  
<sup>322</sup> was used where the main144 code of the examples section was utilized to enable  
<sup>323</sup> the facility to parse input files and provide yoda output files that are using the  
<sup>324</sup> RIVET analysis codes for the data sets specified below. RIVET4.0.1 was used for  
<sup>325</sup> the analysis codes, Rivet plotting and the actual data yoda files. A few significant  
<sup>326</sup> exceptions to this are that the most recent Belle measurements for light and charmed  
<sup>327</sup> mesons [3] were not available yet, therefore yoda data files, Rivet analysis codes  
<sup>328</sup> and plotting instructions were created personally to include them in the tuning.  
<sup>329</sup> Similarly, a few issues were found in the official RIVET codes that were fixed locally.  
<sup>330</sup> Those include a switching of the ordering of integrated hyperon and charmed baryon  
<sup>331</sup> cross sections relative to those differential in the momentum fraction. Also for the  
<sup>332</sup> transverse momentum dependent measurements, the fractional energy  $z$  binning in  
<sup>333</sup> the codes was off by one bin for protons that would be physically impossible to  
<sup>334</sup> cover at Belle energies due to its mass. Also for some measurements the treatment  
<sup>335</sup> of weak decays was inaccurate as only charmed decays were removed in the RIVET  
<sup>336</sup> codes while other weak decays were kept, in contrast to the actual measurements.  
<sup>337</sup> Therefore the weak-decay removed measurements that include pions or protons were  
<sup>338</sup> not included in the fitting procedure. The tune optimization was performed using  
<sup>339</sup> the Professor2.5 package [4].

### <sup>340</sup> **4 Data sets used in the fitting**

<sup>341</sup> For the fitting, the following measurements were used, ordered by publication time:

#### <sup>342</sup> **4.1 BELLE\_2017\_I1606201**

<sup>343</sup> These measurements include various hyperon and charmed baryon final states as  
<sup>344</sup> a function of the fractional momentum  $x_p$  and the total production cross sections  
<sup>345</sup> [5]. Because of these, these measurements are particularly sensitive to the Baryon  
<sup>346</sup> production related PYTHIA variables.

#### <sup>347</sup> **4.2 BELLE\_2017\_I1607562**

<sup>348</sup> These measurements contain the invariant mass and fractional energy dependent  
<sup>349</sup> cross sections for same and opposite charged pairs of pions and kaons within the  
<sup>350</sup> same hemisphere [6]. As such, they provide information on the various mass peaks  
<sup>351</sup> in their range and therefore also indirectly on higher spin and orbital momentum  
<sup>352</sup> particles that feed into these spectra.

<sup>353</sup> **4.3 BELLE\_2019\_I1718551**

<sup>354</sup> These measurements contain the cross sections of pions, kaons and protons as a  
<sup>355</sup> function of energy fraction  $z$  and transverse momentum relative to the thrust axis,  
<sup>356</sup> in bins of the thrust value [7]. Therefore they are most sensitive to the transverse  
<sup>357</sup> momentum generation in the fragmentation, but indirectly also the main LUND  
<sup>358</sup> related fragmentation variables, etc.

<sup>359</sup> **4.4 BELLE\_2020\_I1777678**

<sup>360</sup> In this publication the cross sections as a function of fractional energy  $z$  for pions,  
<sup>361</sup> kaons and protons are included, being likely sensitive to the main Lund fragmenta-  
<sup>362</sup> tion parameters, as well as the baryon related ones for the protons [8]. Additionally,  
<sup>363</sup> also pairs of pions or kaons in same or opposite hemispheres as well as any pairs are  
<sup>364</sup> measured as function of the fractional energies of each hadron. Apart from the nom-  
<sup>365</sup> inal fractional energy definition two alternate definitions are also included, however  
<sup>366</sup> for this exercise they were not included in the tuning effort since those would be  
<sup>367</sup> mostly redundant.

<sup>368</sup> **4.5 BELLE\_2024\_I2849895**

<sup>369</sup> This is the newest result, just published earlier in 2025, and contains a larger number  
<sup>370</sup> of cross sections differential in the momentum fraction  $x_p$  for various lighter and  
<sup>371</sup> charmed mesons decaying into two or three pions or kaons, many for the first time  
<sup>372</sup> at B factories [3]. This data set is most sensitive to the pseudo-scalar to vector-  
<sup>373</sup> meson ratios, the  $\eta$  suppression, the light pseudo-scalar and vector mixing angles,  
<sup>374</sup> and indirectly also the higher spin resonances.

<sup>375</sup> **5 Sample generation, etc**

<sup>376</sup> Given that the number of datasets that are used are very large, it was not possible  
<sup>377</sup> to fit all tuning parameters at the same time. Instead, parameter sets of 6 to 8  
<sup>378</sup> were optimized simultaneously while iterating over all relevant parameters and pre-  
<sup>379</sup> forming the optimization many times to avoid running into local minima. In each  
<sup>380</sup> iteration the best values of the previous tune were set while the next set of variables  
<sup>381</sup> were allowed to float. In the initial iterations the parameter ranges were mostly  
<sup>382</sup> identical to the allowed ranges in PYTHIA while in the later iterations, the ranges  
<sup>383</sup> were narrowed down somewhat for variables that were very stable over the previous  
<sup>384</sup> steps. In PROFESSOR, the initial configurations are randomly created based on the  
<sup>385</sup> boundaries of the variables to optimize using the command *prof2-sample*. In earlier  
<sup>386</sup> iterations about 500 to 1000 samples were generated while in the later stages 2000  
<sup>387</sup> samples were generated. This ensured that the interpolation of the parameter tunes  
<sup>388</sup> and responses could be performed using 5th order polynomials, still. For each sample  
<sup>389</sup> initially 1.2 M and later 5 M  $e^+e^- \rightarrow q\bar{q}$  events were generated for uds and charm  
<sup>390</sup> flavors together. As all these measurements had already been corrected for non- $q\bar{q}$

Table 1: Parameters used in the tuning, their PYTHIA8.3 default values, the BelleII default values (as of release-09-00-01 in generators/modules/fragmentation/-data/pythia\_belle2.charm.dat), empty if PYTHIA 8.2 default value is used, the best value after the tuning and a brief explanation of the parameter.

Variable	P8.3	Belle2	Best	description
<b>StringZ:aLund</b>	<b>0.68</b>	<b>0.32</b>	<b>0.525</b>	<b>(1-z) power</b>
StringZ:bLund	0.98	0.62	0.910	Transverse mass term
StringPT:sigma	0.335		0.372	Transverse momentum in fragmentation
StringFlav:probStoUD	0.217	0.286	0.240	Strangeness suppression wrt to ud quarks
StringFlav:etaSup	0.60		0.850	Extra eta suppression
StringFragmentation:stopMass	1.0	0.3	0.831	Stop mass (End point condition?)
StringFlav:mesonUDVector	0.50		0.554	Vector to PS ratio light quarks
StringFlav:mesonUDL1S0J1	0.0		0.311	Higher spin states L=1, S=0, J=1 light q
StringFlav:mesonUDL1S1J0	0.0		0.236	Higher spin states L=1, S=1, J=0 light q
StringFlav:mesonUDL1S1J1	0.0		0.267	Higher spin states L=1, S=1, J=1 light quarks
StringFlav:mesonUDL1S1J2	0.0		0.400	Higher spin states L=1, S=1, J=2 light quarks
StringFlav:mesonSvector	0.55		0.870	Vector to PS ratio strange quarks
StringFlav:mesonSDL1S0J1	0.0		0.118	Higher spin states L=1, S=0, J=1 s quarks
StringFlav:mesonSDL1S1J0	0.0		0.374	Higher spin states L=1, S=1, J=0 s quarks
StringFlav:mesonSDL1S1J1	0.0		0.365	Higher spin states L=1, S=1, J=1/2 s quarks
StringFlav:mesonSDL1S1J2	0.0		0.588	Higher spin states L=1, S=1, J=1/2 s quarks
StringZ:rFactC	1.32	1.0	0.410	Bowler modification for charm quarks
StringFlav:mesonCvector	0.88	2.8	2.226	Vector to PS ratio charm quarks
StringFlav:mesonCDL1S0J1	0.0	0.06	1.729	Higher spin states L=1, S=0, J=1 charm
StringFlav:mesonCDL1S1J0	0.0	0.1775	0.635	Higher spin states L=1, S=1, J=0 charm
StringFlav:mesonCDL1S1J1	0.0	0.1868	2.644	Higher spin states L=1, S=1, J=1 charm
StringFlav:mesonCDL1S1J2	0.0	0.1836	1.972	Higher spin states L=1, S=1, J=2 charm
StringFlav:thetaPS	-15		-15.71	Mixing angle for PS mesons
StringFlav:thetaV	36		27.08	Mixing angle for V mesons
StringFlav:probQQtoQ	0.081	0.133	0.064	Diquark over quark ratio
StringZ:aExtraDiquark	0.97		1.696	Lund extra a term for diquarks(baryons)
StringFlav:probSQtoQQ	0.9156	0.323	0.521	Strange over light diquark suppression
StringFlav:probQQ1toQQ0	0.0275	0.0468	0.252	Vector over scalar diquark suppression
StringFlav:popcornRate			0.055112	mesons between diquark pairs
StringFlav:popcornSpair			0.106073	strange Popcorn diquark
StringFlav:popcornSmeson			0.447140	strange meson in Popcorn

391 contributions, no other hard processes are included. Also ISR had been corrected in  
 392 the measurements so it was switched off in the MC generation as well.

393 The following sets of parameters were optimized together initially:

- 394 • Set A (main Lund): StringZ:aLund, StringZ:bLund, StringPT:sigma, StringFlav:probStoUD,  
 395 StringFlav:etaSup, StringFragmentation:stopMass
- 396 • Set B (baryons and charm): StringFlav:probQQtoQ, StringFlav:probSQtoQQ,  
 397 StringFlav:probQQ1toQQ0, StringZ:aExtraDiquark, StringZ:rFactC, StringFlav:mesonCvector  
 398 StringFlav:mesonCL1S0J1, StringFlav:mesonCL1S1J0
- 399 • Set C (vector mesons, mixing): StringFlav:mesonUDvector, StringFlav:mesonUDL1S0J1,  
 400 StringFlav:mesonUDL1S1J0, StringFlav:mesonSvector, StringFlav:mesonSL1S0J1,  
 401 StringFlav:mesonSL1S1J0, StringFlav:thetaPS, StringFlav:thetaV
- 402 • Set D (higher spin states): StringFlav:mesonUDL1S1J1, StringFlav:mesonUDL1S1J2,  
 403 StringFlav:mesonSL1S1J1, StringFlav:mesonSL1S1J2, StringFlav:mesonCL1S1J1,

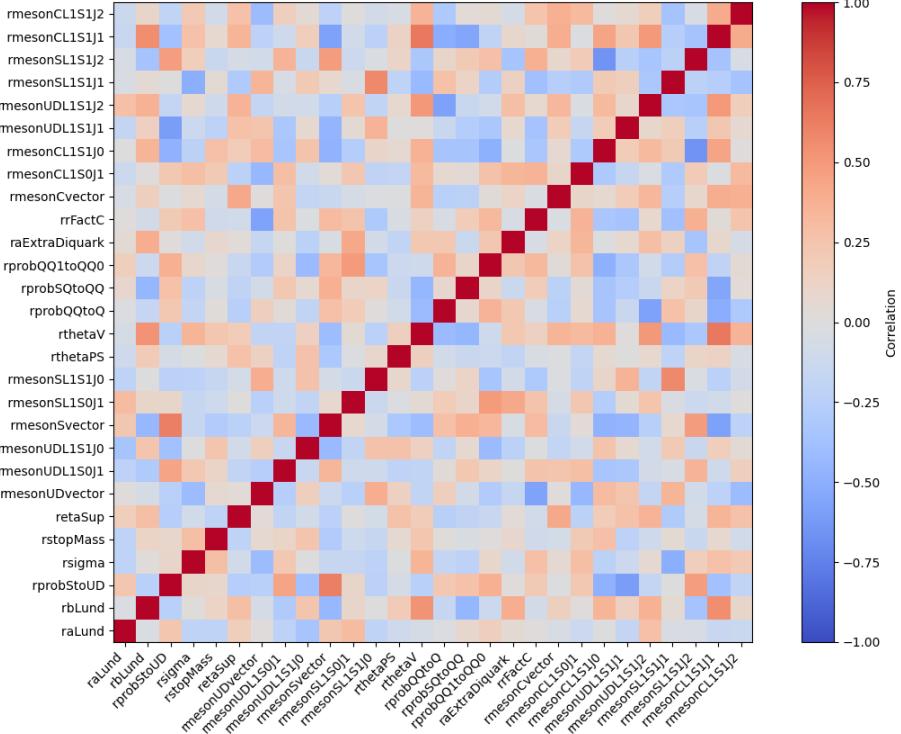


Figure 1: Correlation matrix of all parameters as obtained from a test tuning set that was run over 5000 parameters, a reduced set of data sets and only a third order interpolation in order to be computationally feasible at all.

404      `StringFlav:mesonCL1S1J2`

405      As can be seen in Fig. 1, all these 28 parameters are not uncorrelated, nor do the  
 406      parameters of each set factorize either but generally they are somewhat less corre-  
 407      lated between sets. Because of this an iterative approach was used where sets A to D  
 408      were optimized several times after optimizing each set first (i.e. A → B → C → D → A → B → etc.)  
 409      The individual correlation matrices after the last iteration of each tuning set are  
 410      shown in Fig. 2. As one can see, within a tuning set correlations are more pro-  
 411      nounced, most notably between the main two Lund parameters, but also, to a lesser  
 412      extend between others.

413      At later iterations of the optimization, the more stable variables were retired  
 414      (`StringPT:sigma`, `StringFlav:probStoUD`, `StringFlav:mesonUDvector`, `StringFlav:probQQtoQ`),  
 415      using their best values from then on, but including the additional higher spin states  
 416      and eventually the popcorn variables. The later settings therefore became:

417      • Set A' (main Lund): `StringZ:aLund`, `StringZ:bLund`, `StringFlav:etaSup`, `StringFrag-`  
 418      `mentation:stopMass`, `mesonUDL1S0J1`, `mesonUDL1S1J0`

419      • Set B' (baryons): `StringFlav:probSQtoQQ`, `StringFlav:probQQ1toQQ0`, `StringZ:aExtraDiquark`  
 420      `popcornRate`, `StringFlav:popcornSpair`, `StringFlav:popcornSmeson`

421      • Set C' (strange+mixing): `StringFlav:mesonSvector`, `StringFlav:mesonSL1S0J1`,

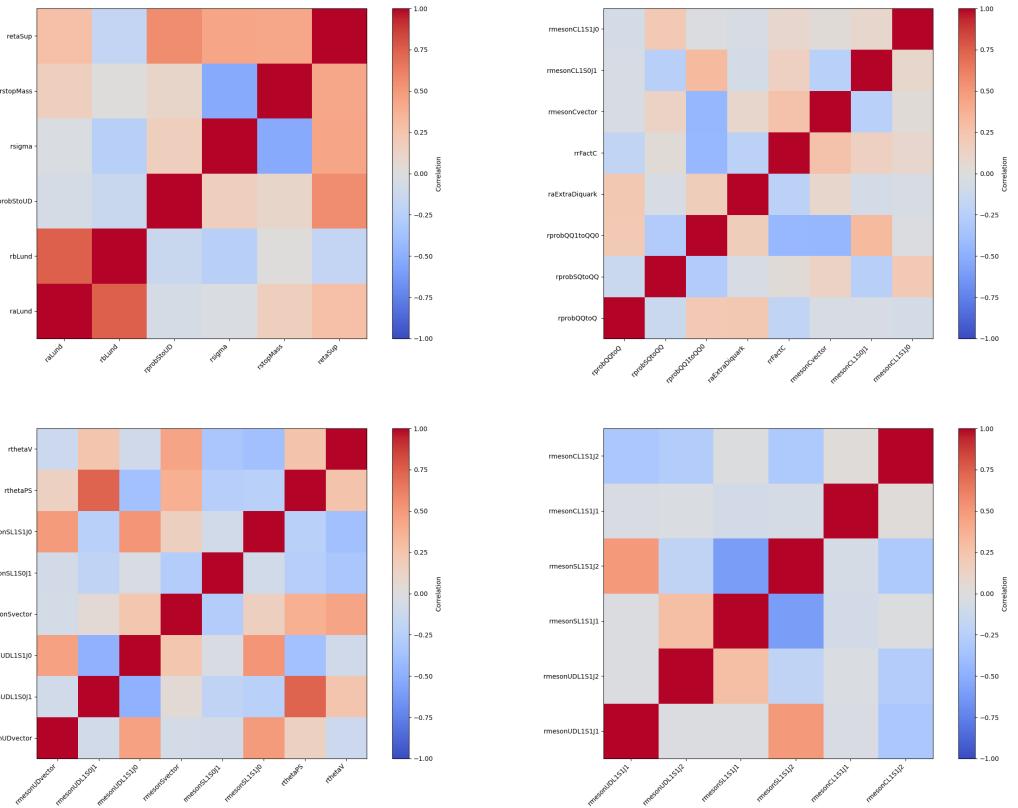


Figure 2: Correlation matrices of each tuning set separately, obtained from the last iterations of the nominal tuning procedure and interpolation based on 2000 parameter sets each, the full data sets and a 5th order polynomial interpolation.

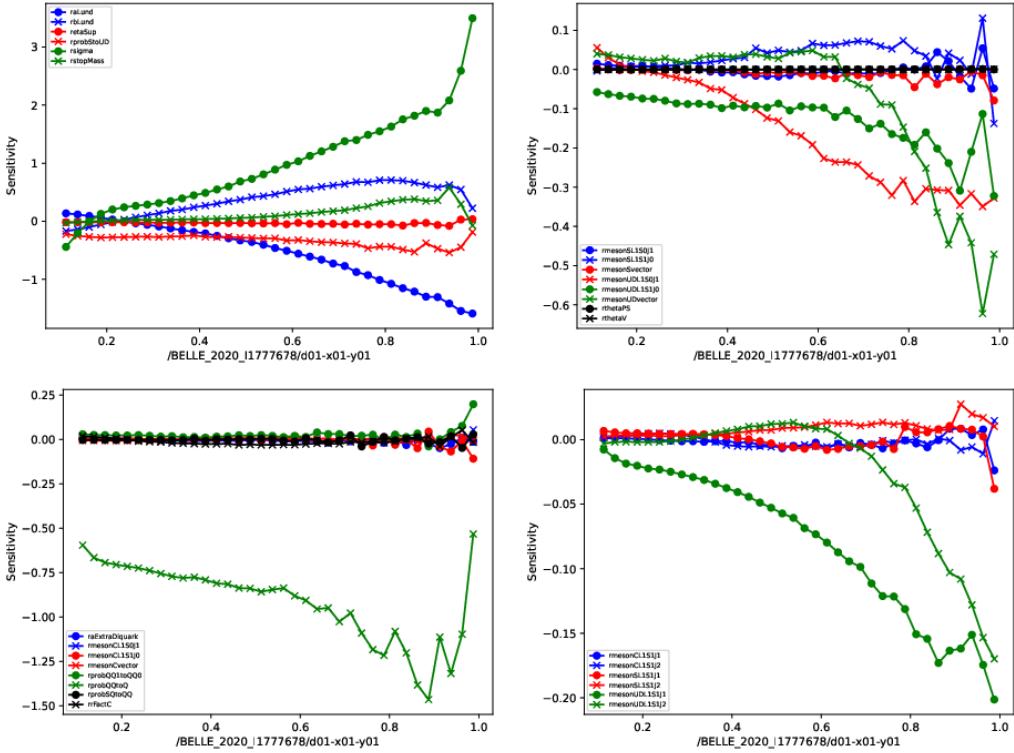


Figure 3: Sensitivities of the pion cross sections as a function of the fractional energy  $z$ . The different curves correspond to the sensitivities to the various tune parameters.

422        StringFlav:mesonSL1S1J0, StringFlav:mesonSL1S1J1, StringFlav:mesonSL1S1J2,  
 423        StringFlav:thetaPS, StringFlav:thetaV

424        • Set D' (charm): StringZ:rFactC, StringFlav:mesonCvector, StringFlav:mesonCL1S0J1,  
 425        StringFlav:mesonCL1S1J0, StringFlav:mesonCL1S1J1, StringFlav:mesonCL1S1J2

## 426        6 Individual sensitivities

427        In the following the individual sensitivities to the various tune parameters are shown  
 428        for several of the key measurements.

### 429        6.1 Single hadron cross sections

430        This single pion cross sections have naturally a very high sensitivity to the main Lund  
 431        fragmentation parameters, as well as to the fragmentation transverse momentum as  
 432        can be seen in Fig. 3. There is also some sensitivity to the light quark vector mesons  
 433        to pseudoscalar ratios and higher spin states. For kaons the sensitivities are similar  
 434        except that strangeness suppression and the corresponding strange quark VM and  
 435        higher spin variables are more sensitive as can be seen in Fig. 4. Protons in contrast  
 436        are mostly sensitive to the diquark ratio and to a lesser extend the main Lund  
 437        parameters.

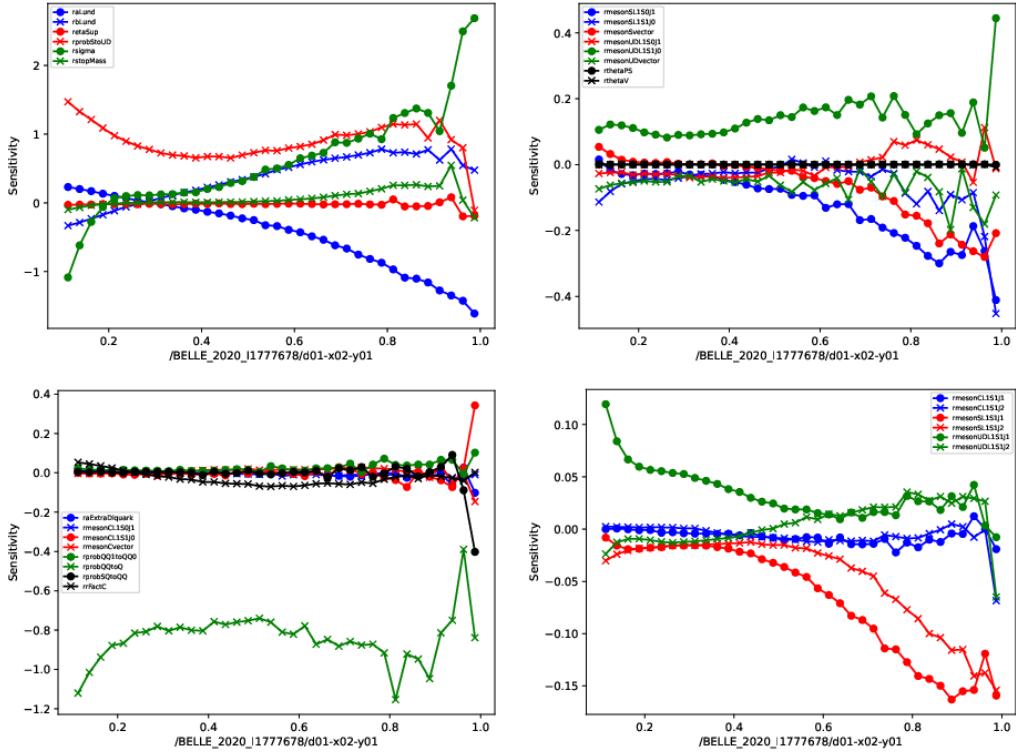


Figure 4: Sensitivities of the kaon cross sections as a function of the fractional energy  $z$ . The different curves correspond to the sensitivities to the various tune parameters.

438 For the vector mesons cross sections, the vector mesons variables for the relevant  
 439 flavors are clearly the most sensitive parameters as can be seen in Fig. 6 for the  $\rho$   
 440 mesons, Fig. 7 for the  $\omega$  Fig. 8, for the  $K^*$  and Fig. 9 for the  $\phi$  mesons. The strange  
 441 mesons do also have some sensitivity to the strangeness suppression again.

442 The  $\eta$  mesons naturally are most sensitive to the eta suppression parameter while  
 443 they also provide a small sensitivity to the pseudoscalar mixing angle, apart from  
 444 the regular Lund parameters, as shown in Fig. 10.

445 The charmed mesons obtain additional sensitivity to the extra charm term for  
 446 the fragmentation, as well as for the vector mesons to the charmed VM hand higher  
 447 spin state variables.

## 448 6.2 Di-hadron cross sections

449 For the di-hadron cross sections, again the vector mesons components appear in  
 450 the vicinity of their masses, while additionally some sensitivity to the higher spin  
 451 mesons is visible, particularly at higher masses as those can mostly be only indirectly  
 452 obtained in these di-hadron spectra.

## 453 6.3 Transverse momentum dependent cross sections

454 The transverse momentum dependent cross sections naturally have a very high sen-  
 455 sitivity to the transverse momentum generated in the fragmentation process as can

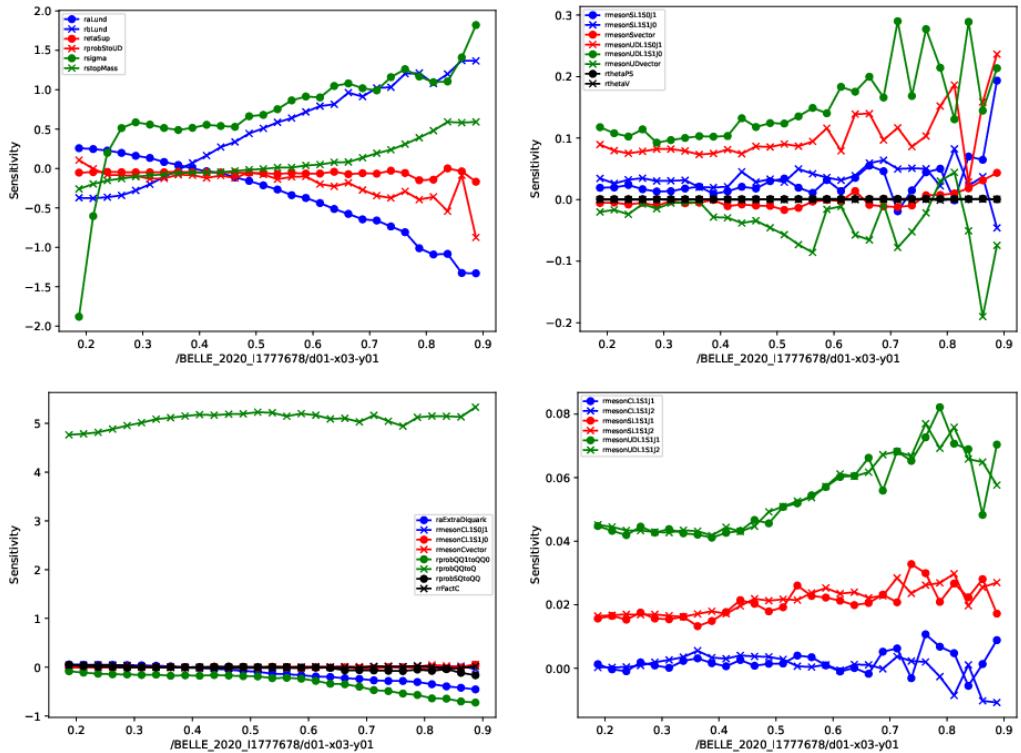


Figure 5: Sensitivities of the proton cross sections as a function of the fractional energy  $z$ . The different curves correspond to the sensitivities to the various tune parameters.

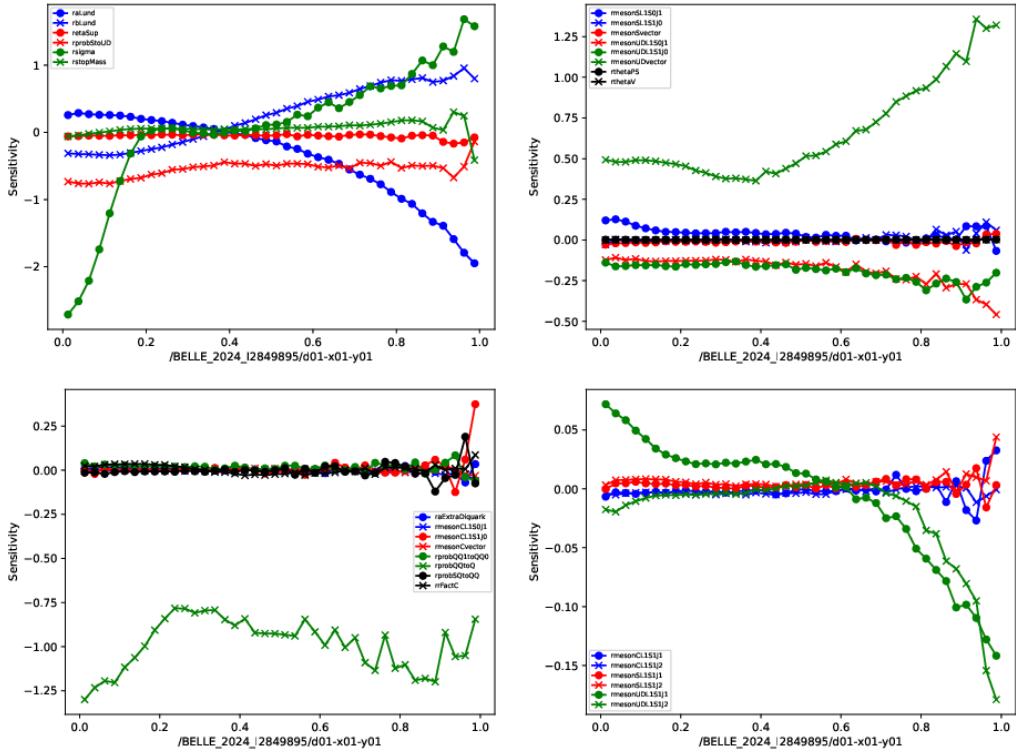


Figure 6: Sensitivities of the  $\rho^0$  cross sections as a function of the fractional energy  $x_p$ . The different curves correspond to the sensitivities to the various tune parameters.

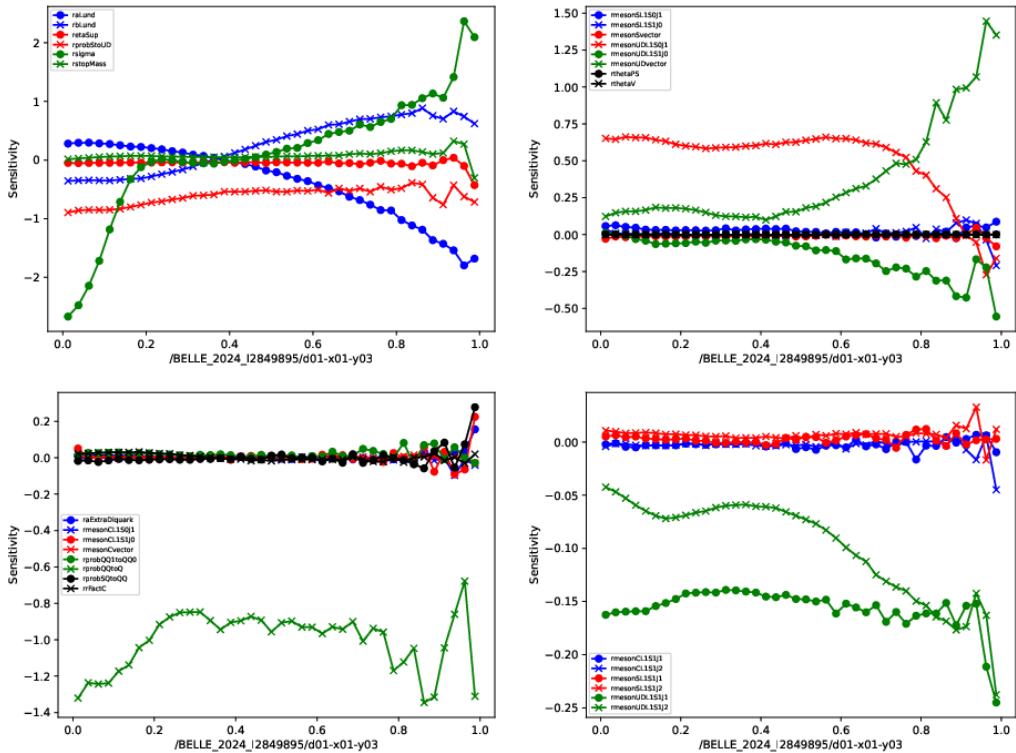


Figure 7: Sensitivities of the  $\omega$  cross sections as a function of the fractional energy  $x_p$ . The different curves correspond to the sensitivities to the various tune parameters.

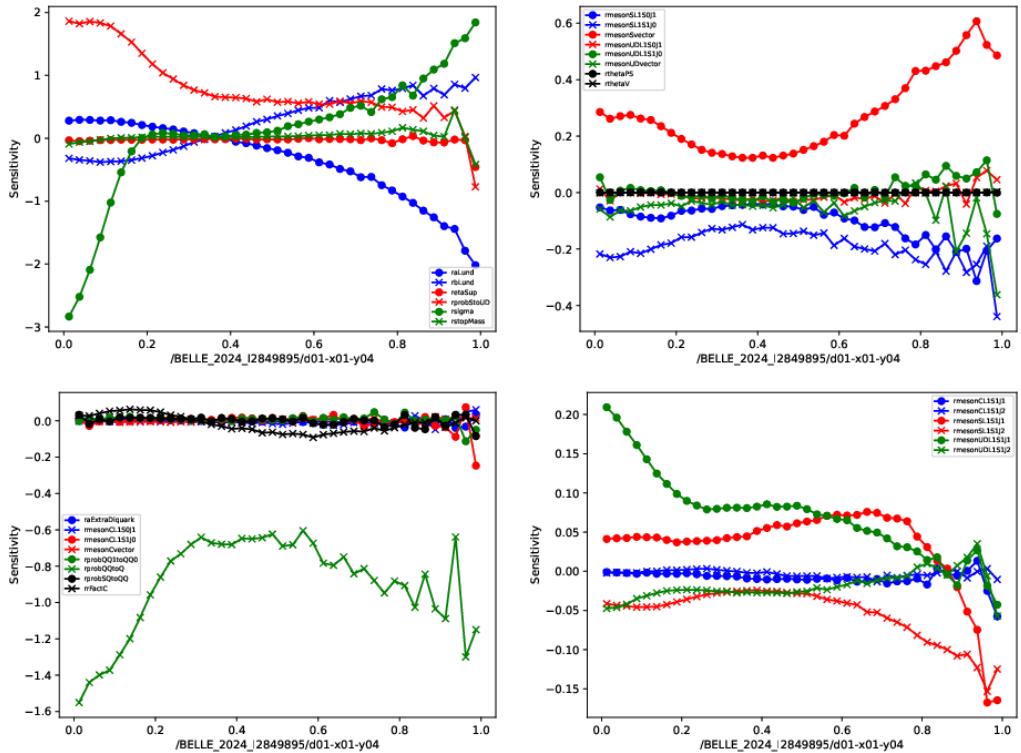


Figure 8: Sensitivities of the  $K^{*0}$  cross sections as a function of the fractional energy  $x_p$ . The different curves correspond to the sensitivities to the various tune parameters.

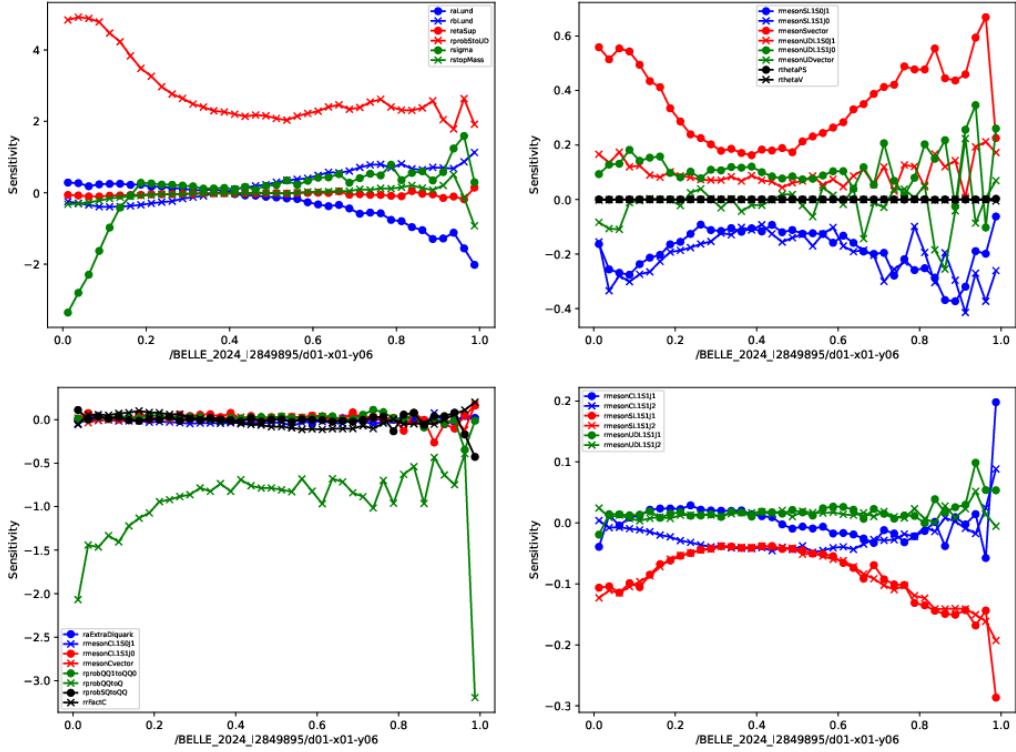


Figure 9: Sensitivities of the  $\phi$  cross sections as a function of the fractional energy  $x_p$ . The different curves correspond to the sensitivities to the various tune parameters.

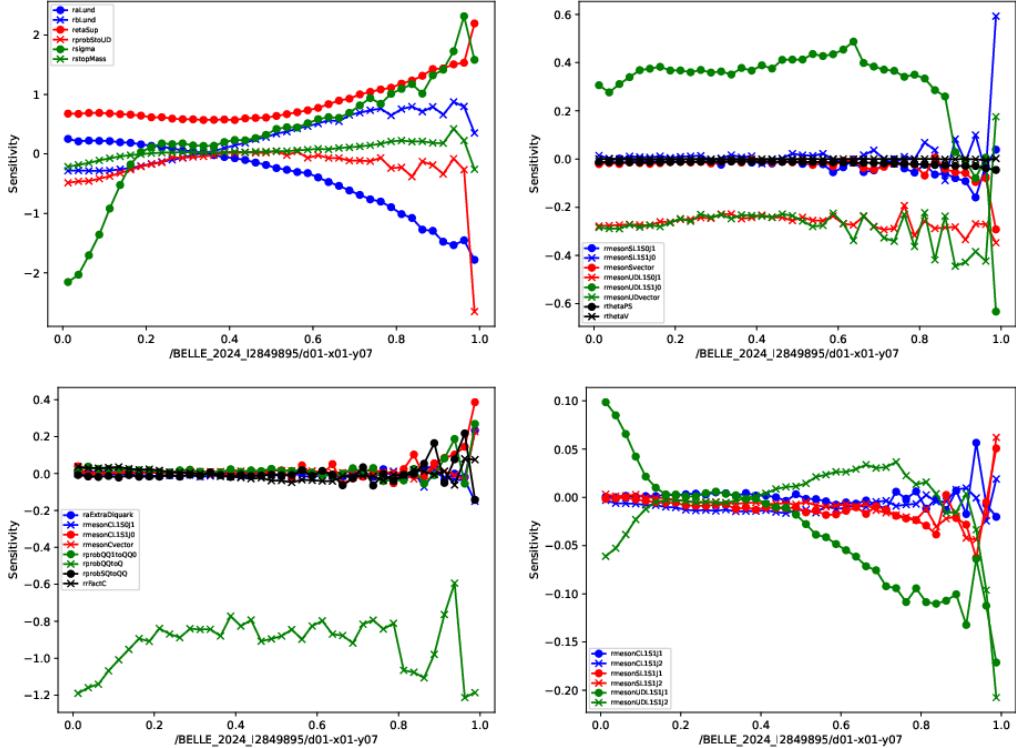


Figure 10: Sensitivities of the  $\eta$  cross sections as a function of the fractional energy  $x_p$ . The different curves correspond to the sensitivities to the various tune parameters.

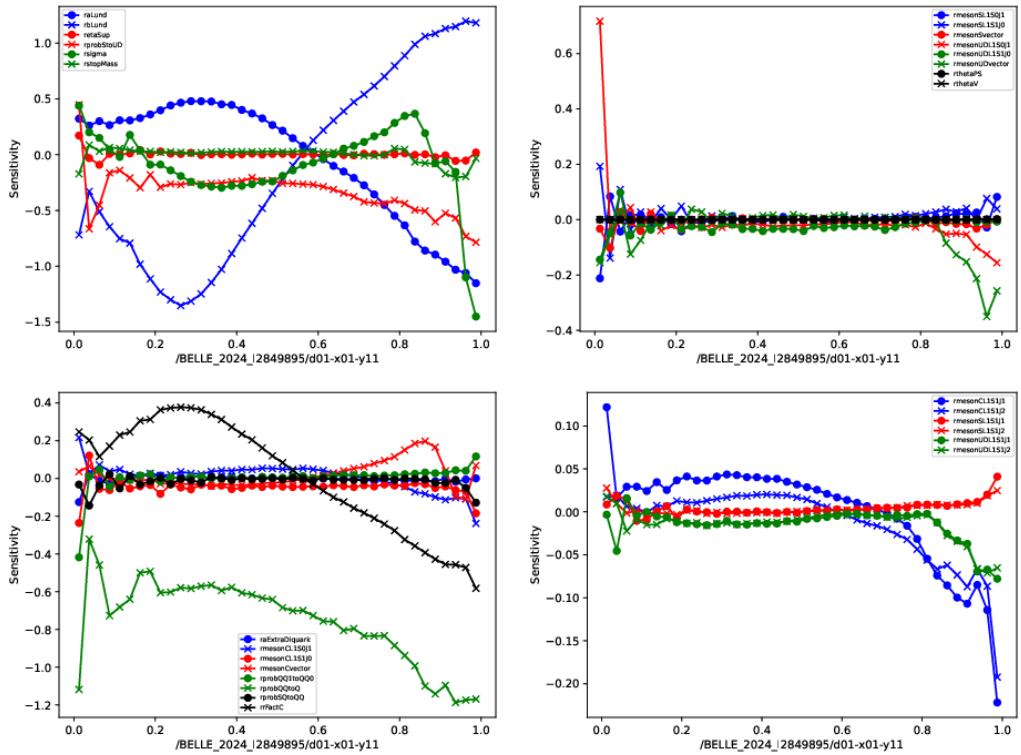


Figure 11: Sensitivities of the  $D^+$  cross sections as a function of the fractional energy  $x_p$ . The different curves correspond to the sensitivities to the various tune parameters.

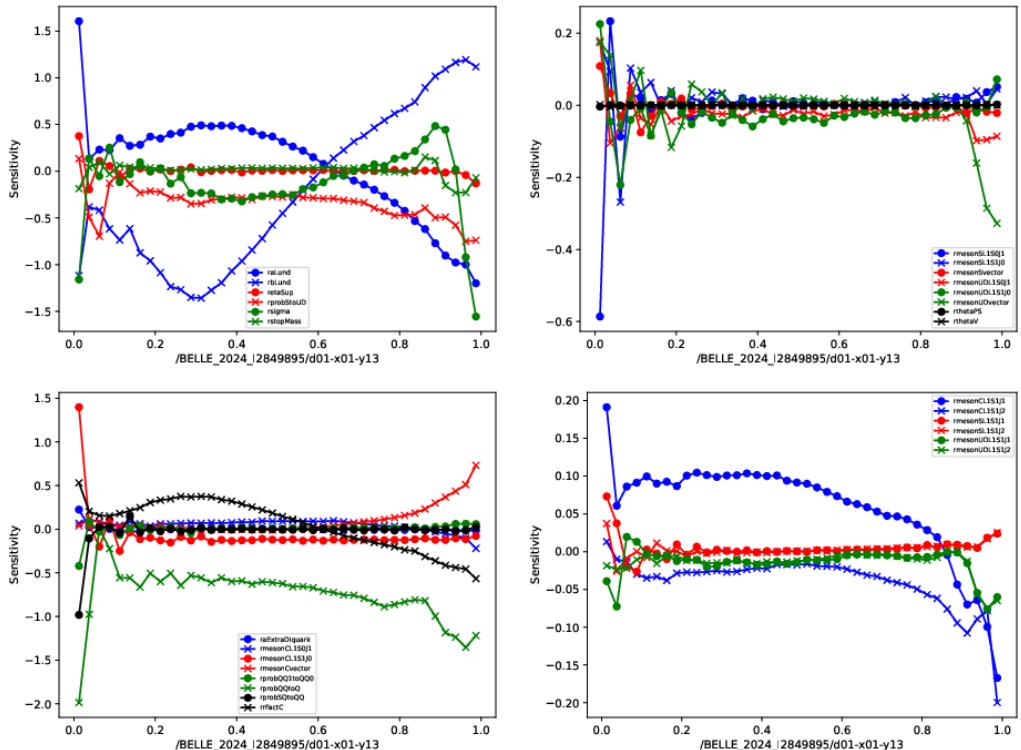


Figure 12: Sensitivities of the  $D^{*0}$  cross sections as a function of the fractional energy  $x_p$ . The different curves correspond to the sensitivities to the various tune parameters.

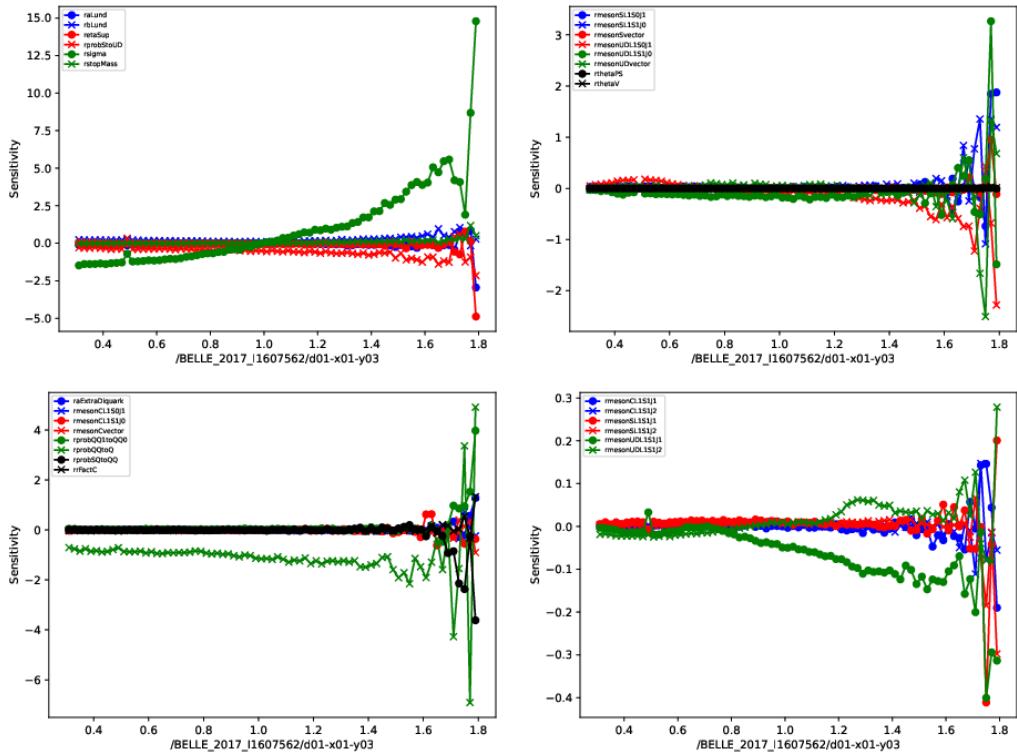


Figure 13: Sensitivities of the  $\pi^+\pi^-$  cross sections as a function of the invariant mass, in the  $z$  bin. The different curves correspond to the sensitivities to the various tune parameters.

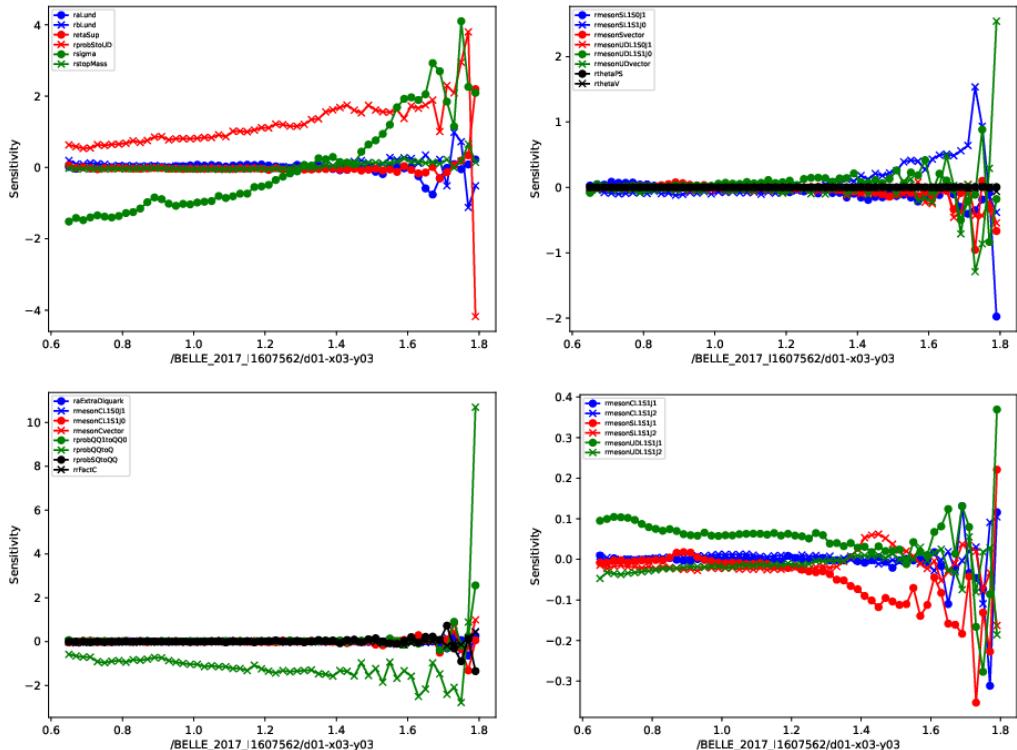


Figure 14: Sensitivities of the  $\pi^+K^-$  cross sections as a function of the invariant mass, in the  $z$  bin. The different curves correspond to the sensitivities to the various tune parameters.

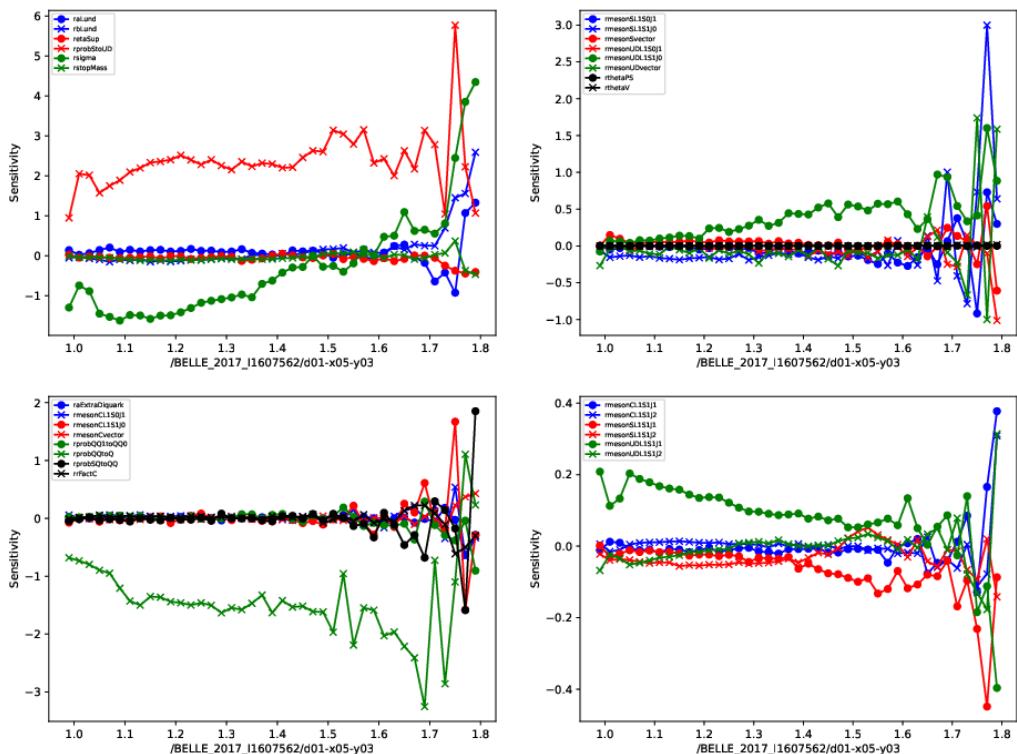


Figure 15: Sensitivities of the  $K^+K^-$  cross sections as a function of the invariant mass, in the  $z$  bin. The different curves correspond to the sensitivities to the various tune parameters.

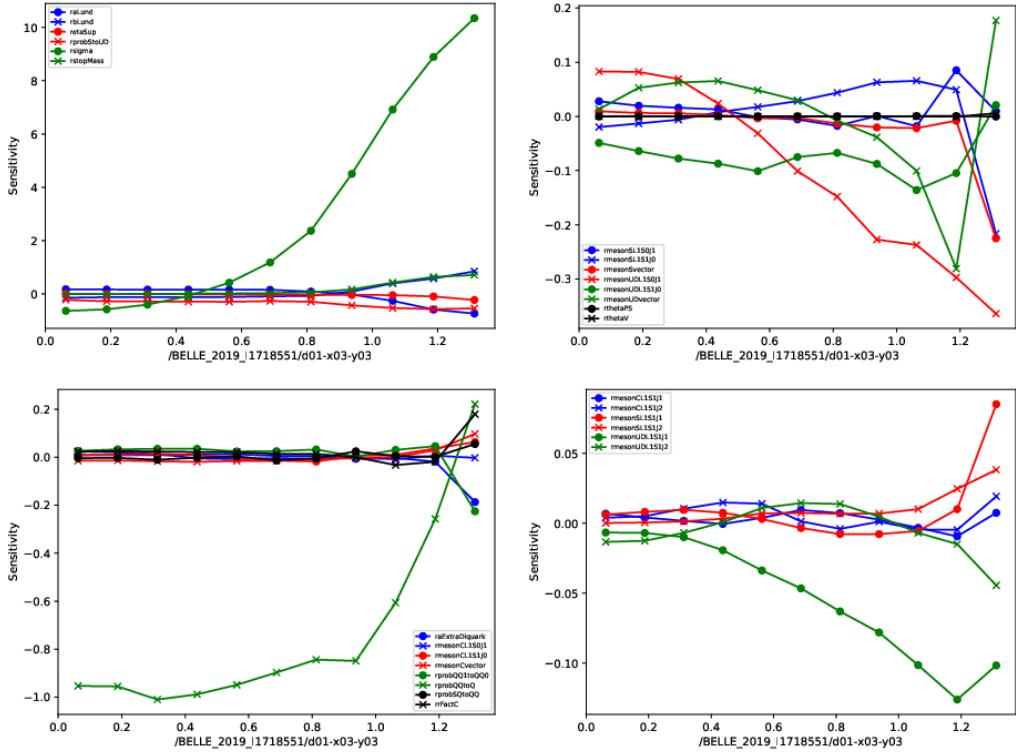


Figure 16: Sensitivities of the  $\pi$  cross sections as a function of the transverse momentum in the  $z$  bin and a thrust value of  $0.8 - 0.9$ . The different curves correspond to the sensitivities to the various tune parameters.

456 be seen in Figs. 16 to 18.

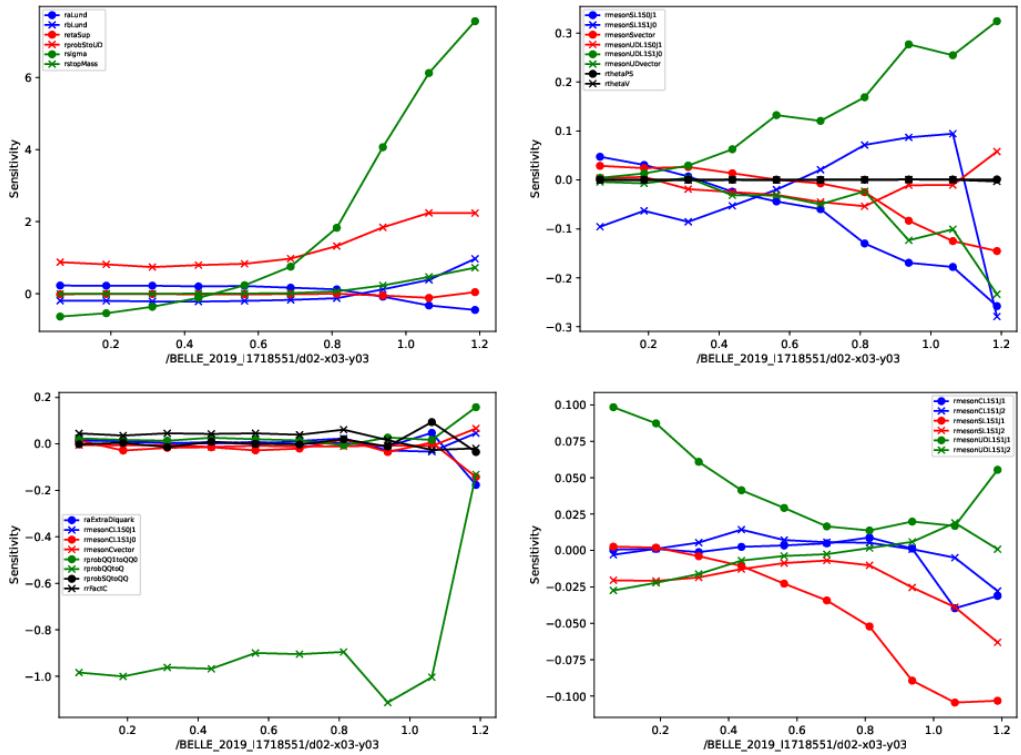


Figure 17: Sensitivities of the  $\pi$  cross sections as a function of the transverse momentum in the  $z$  bin and a thrust value of  $0.8 - 0.9$ . The different curves correspond to the sensitivities to the various tune parameters.

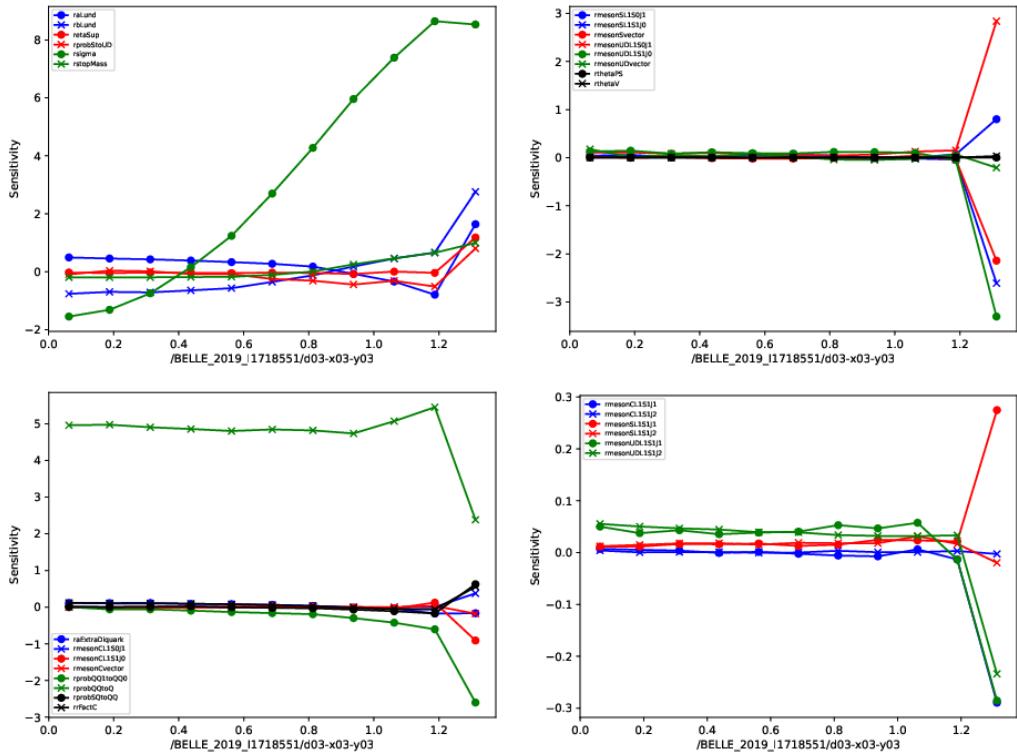


Figure 18: Sensitivities of the  $\pi$  cross sections as a function of the transverse momentum in the  $z$  bin and a thrust value of  $0.8 - 0.9$ . The different curves correspond to the sensitivities to the various tune parameters.

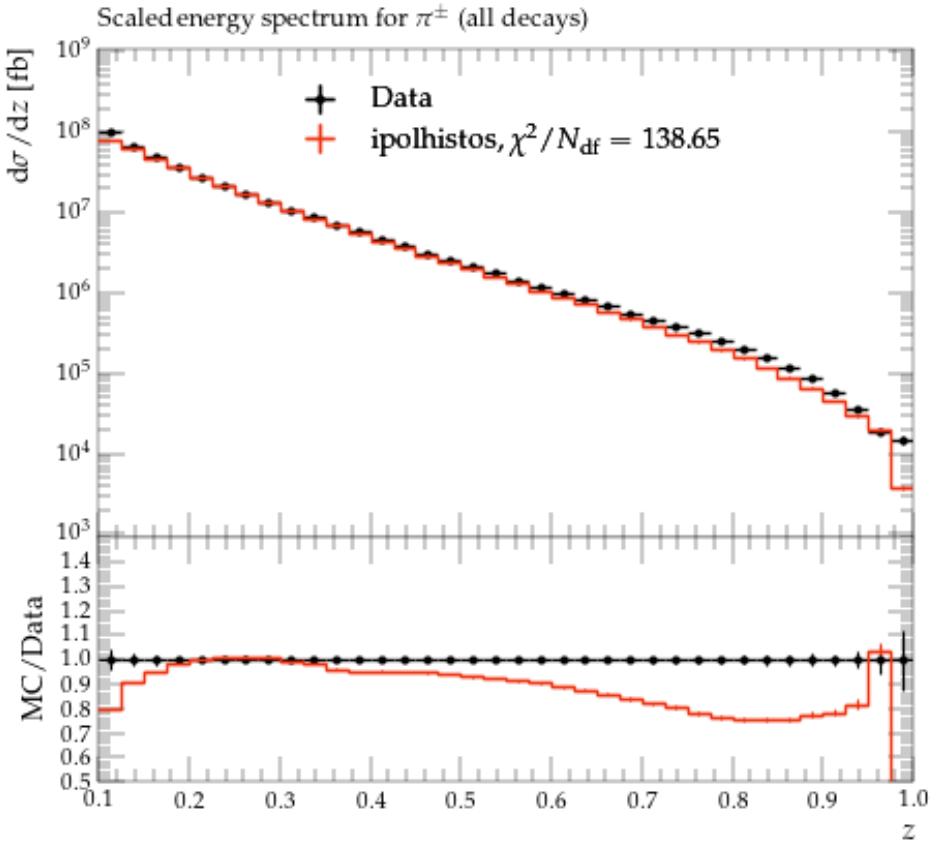


Figure 19: Pion cross sections as a function of the fractional energy  $z$ . The data is displayed by black points while the best fit result in red.

## 457 7 Tuning fits

### 458 7.1 Main hadrons

459 The best results can be seen in Fig. 19 to 21 for the main pion, kaon and proton  
 460 cross sections. One can see that for the mesons the data can be described reasonably  
 461 well overall, while the high precision of the pion data still results in fairly high  $\chi^2$ .  
 462 The proton data cannot be described so well which appears to be a common problem  
 463 for baryon production in the Lund model as will be apparent from the other baryon  
 464 related results below.

### 465 7.2 Decaying and charmed mesons

466 For the various light mesons that were studied in publication [3], the tuning efforts  
 467 are able to provide a good description of the data and generally low  $\chi^2$ . Those fit  
 468 results are displayed in Figs. 22 to 25.

469 Charmed mesons are also mostly well described, with the vector mesons compar-  
 470 ing particularly well, as can be seen in Figs. 26 to 28. On the strange D mesons are  
 471 slightly less well described as apparently the additional shift in the peak positions  
 472 due to the heavier strange quarks cannot be well accommodated in the Lund model.

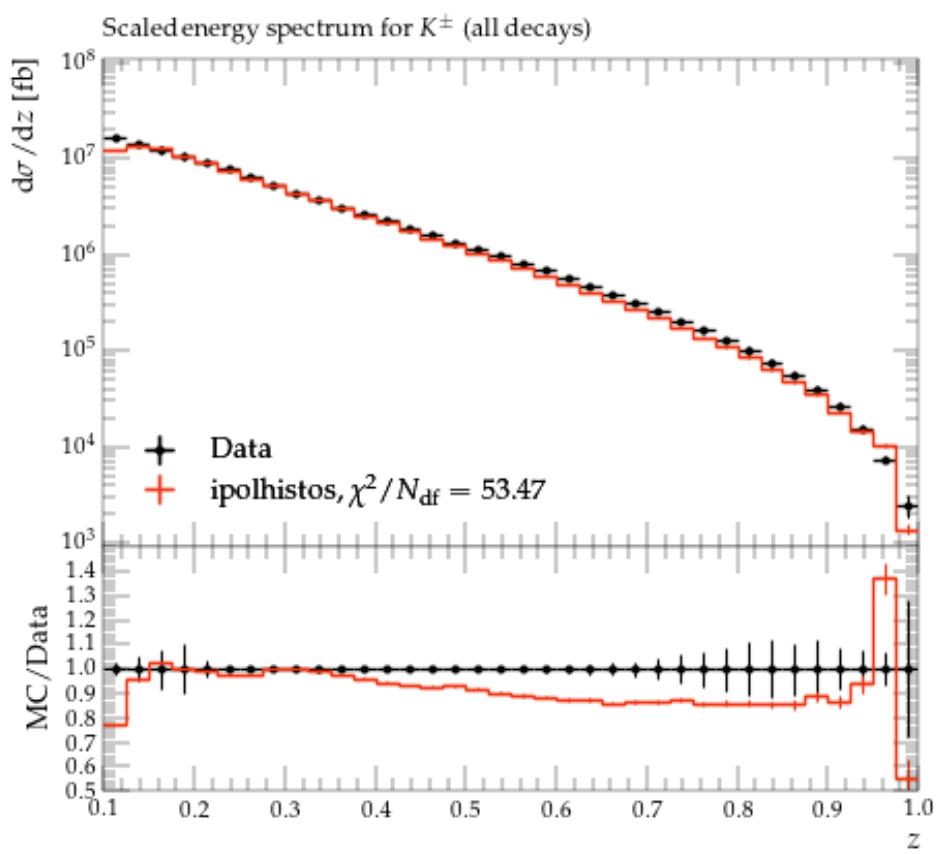


Figure 20: Kaon cross sections as a function of the fractional energy  $z$ . The data is displayed by black points while the best fit result in red.

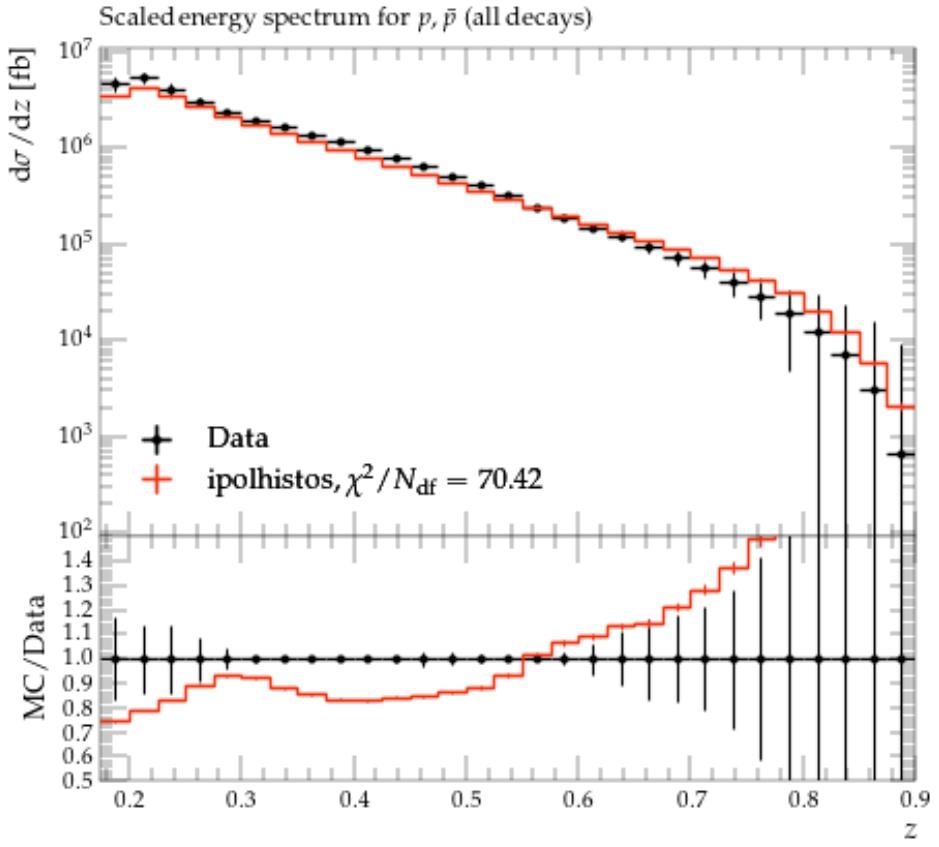


Figure 21: Proton cross sections as a function of the fractional energy  $z$ . The data is displayed by black points while the best fit result in red.

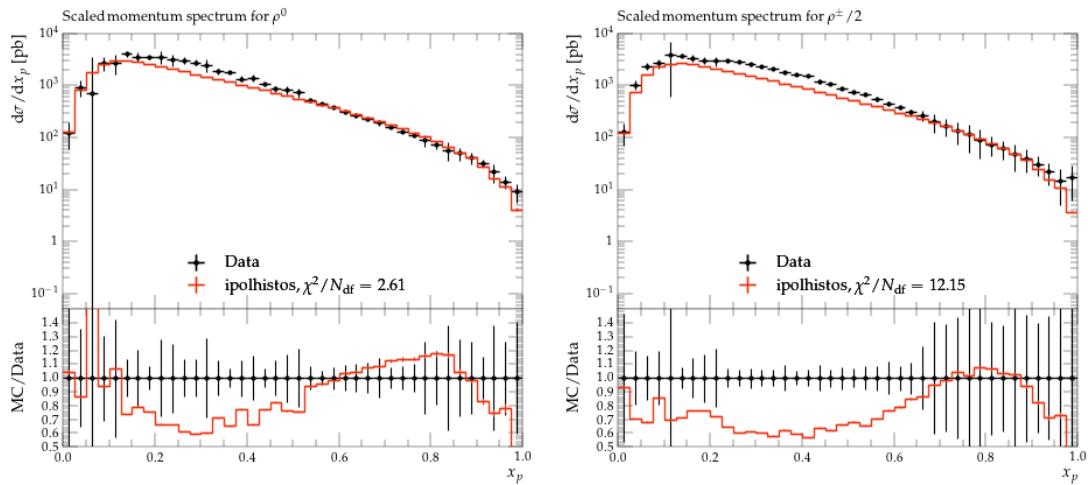


Figure 22: Left: neutral  $\rho$  cross sections as a function of the fractional momentum  $x_p$ . Right: charged  $\rho$  cross sections. The data is displayed by black points while the best fit result in red.

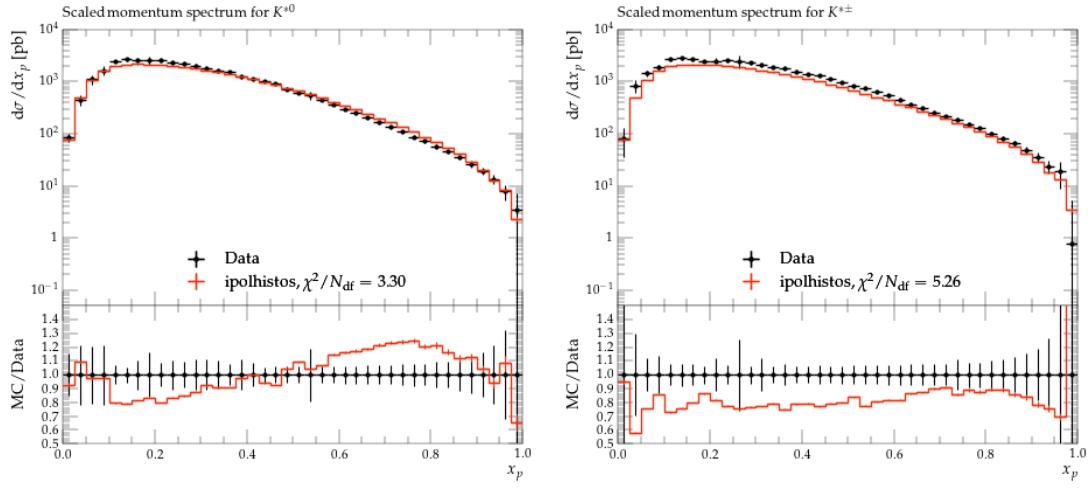


Figure 23: Left: neutral  $K^*$  cross sections as a function of the fractional momentum  $x_p$ . Right: charged  $K^*$  cross sections. The data is displayed by black points while the best fit result in red.

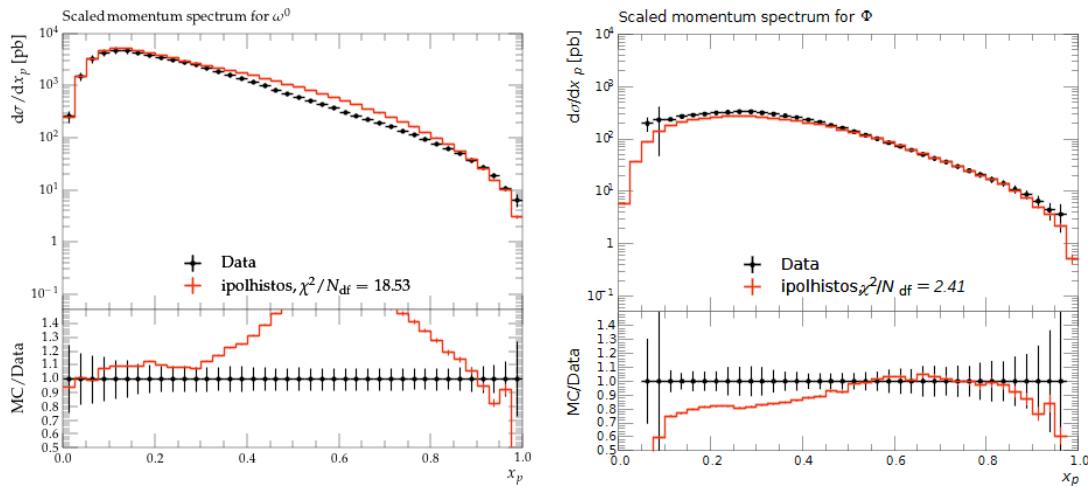


Figure 24: Left:  $\omega$  cross sections as a function of the fractional momentum  $x_p$ . Right:  $\phi$  cross sections. The data is displayed by black points while the best fit result in red. The missing  $\chi^2$  is 3.96.

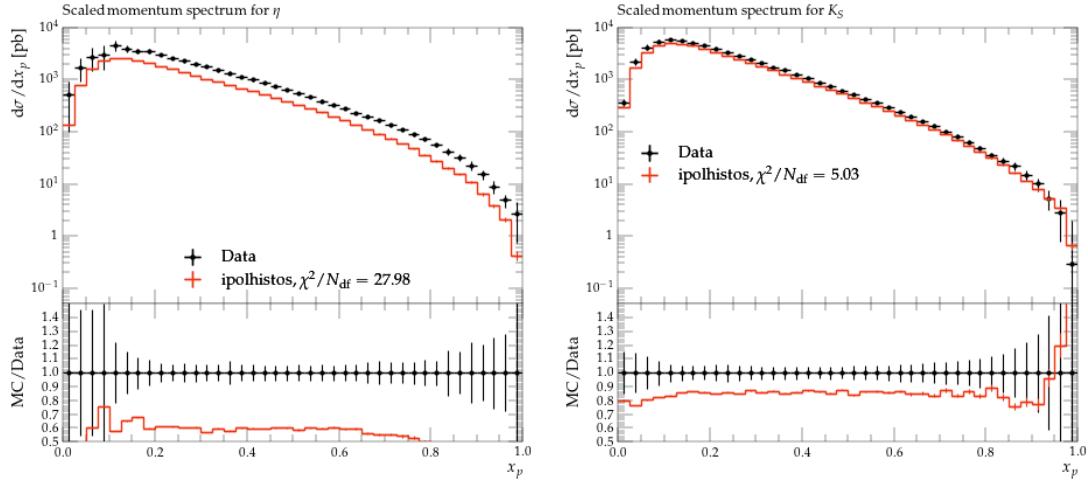


Figure 25: Left:  $\eta$  cross sections as a function of the fractional momentum  $x_p$ . Right:  $K_S$  cross sections. The data is displayed by black points while the best fit result in red.

<sup>473</sup> In the figures the  $\chi^2$  values are often given as nans, since Rivet cannot deal with  
<sup>474</sup> empty bins, but they were added by hand based on the professor tuning outcome  
<sup>475</sup> which does provide them correctly.

### <sup>476</sup> 7.3 Di-hadrons in various configurations

<sup>477</sup> In the following, examples of the dihadron invariant mass distributions are shown  
<sup>478</sup> for one low and one higher fractional energy bin in Figs. 29 to 34. One can see that  
<sup>479</sup> for many hadron combinations, the overall description is good, but some features  
<sup>480</sup> are not well reproduced. Most notably in the opposite-sign pion-kaon spectra the  
<sup>481</sup> bump at around 1.5 GeV is not as pronounced in the MC, or rather somewhat  
<sup>482</sup> elongated in comparison to the data. As the underlying decay of D mesons into  
<sup>483</sup>  $K\pi\pi$  is also present in PYTHIA, likely some of the details are not as well described  
<sup>484</sup> there compared to EvtGen (as the bump was very clearly visible in the Belle I MC  
<sup>485</sup> as well). Another aspect that is not well described are the same-sign pion pair's low  
<sup>486</sup> mass region which generally underestimates the amount of pairs. For pion-kaon and  
<sup>487</sup> kaon pairs the description is generally quite resonable also at lower masses.

<sup>488</sup> Also the back-to-back di-hadron distributions as a function of fractional energies,  
<sup>489</sup> the description of the data by the best tune is again very reasonable, as shown in  
<sup>490</sup> Figs. 35 to 40 for selected fractional energy bin and hadron type combinations.

### <sup>491</sup> 7.4 Transverse momentum dependent cross sections

<sup>492</sup> The transverse momentum dependent cross sections are also fairly well described,  
<sup>493</sup> particularly the low transverse momentum region that most directly is sensitive to  
<sup>494</sup> the transverse momentum generated in the fragmentation process. In the higher  
<sup>495</sup> transverse momentum tails, some slight differences can be seen, albeit with rather  
<sup>496</sup> large uncertainties on the measurements.

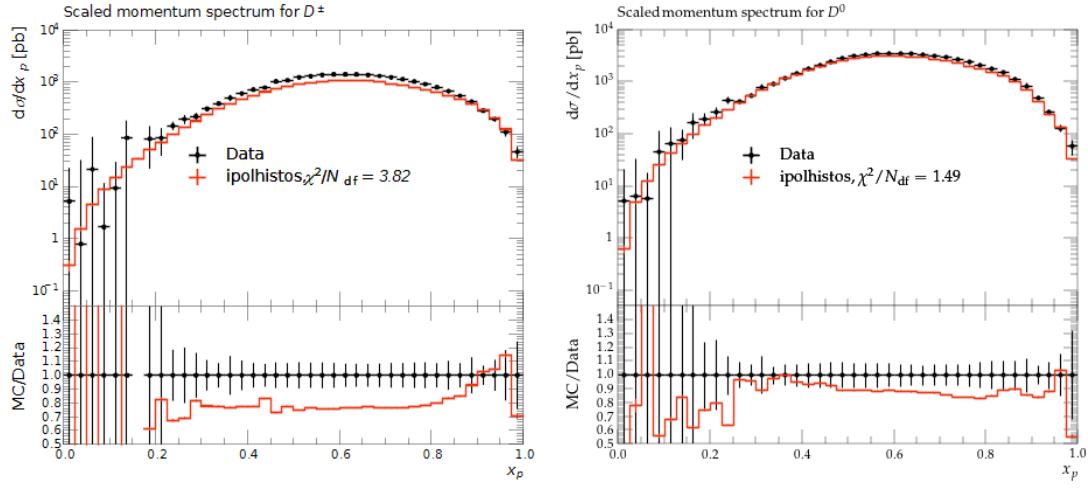


Figure 26: Left:  $D^+$  cross sections as a function of the fractional momentum  $x_p$ . Right:  $D^0$  cross sections. The data is displayed by black points while the best fit result in red.

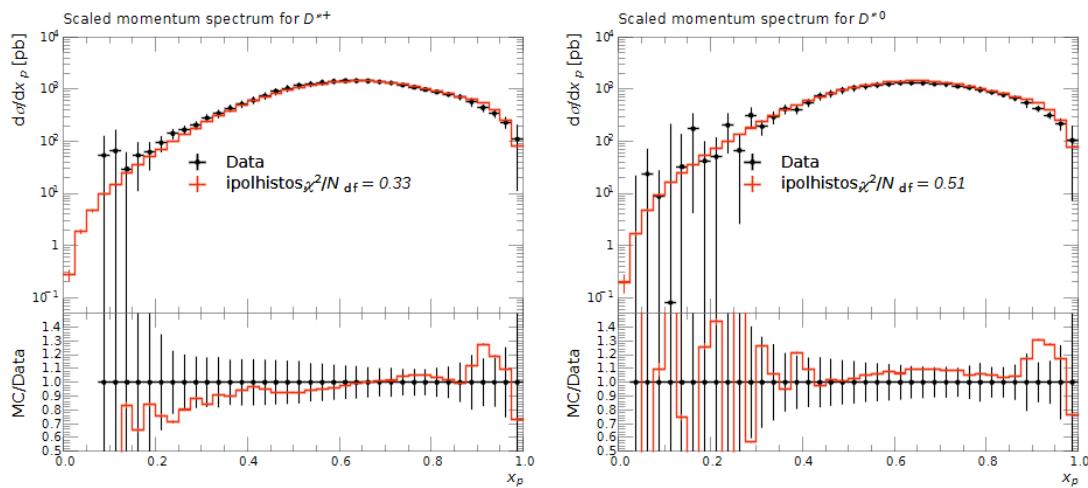


Figure 27: Left:  $D^{*+}$  cross sections as a function of the fractional momentum  $x_p$ . Right:  $D^{*0}$  cross sections. The data is displayed by black points while the best fit result in red.

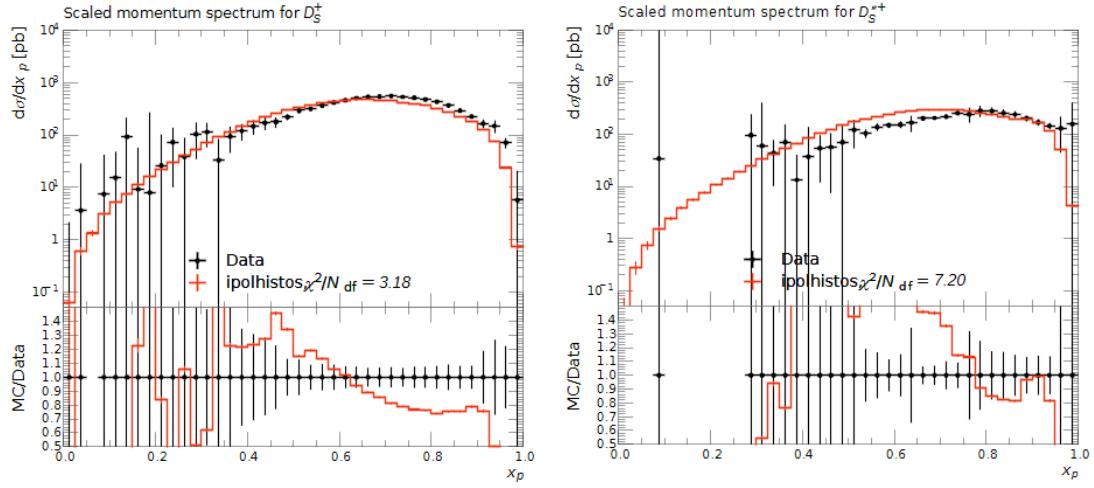


Figure 28: Left:  $D_s^+$  cross sections as a function of the fractional momentum  $x_p$ . Right:  $D_s^{*+}$  cross sections. The data is displayed by black points while the best fit result in red.

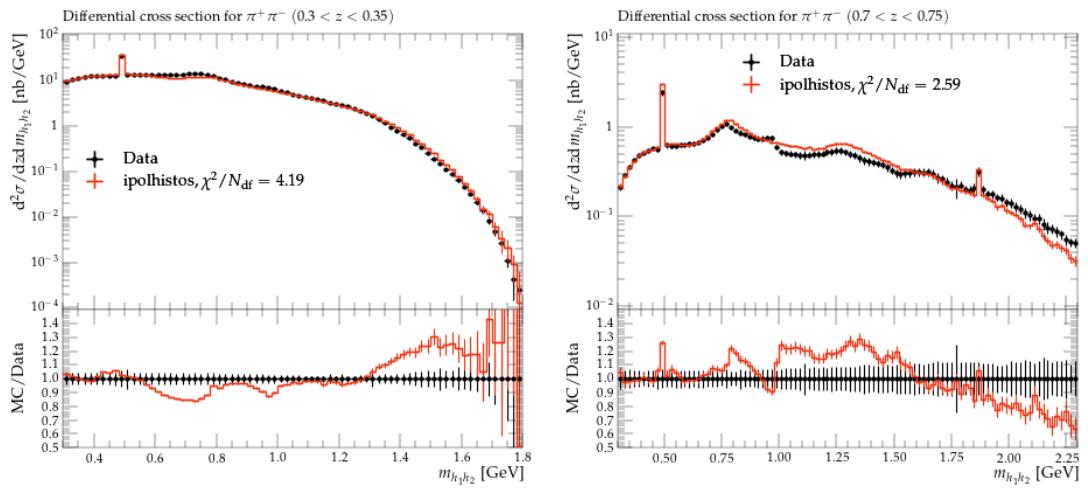


Figure 29: Left:  $\pi^+\pi^-$  pair cross sections as a function of the invariant mass  $m$  for the fractional energy bin  $0.3 - 0.35$ . Right: The same for the fractional energy bin  $0.7 - 0.75$ . The data is displayed by black points while the best fit result in red.

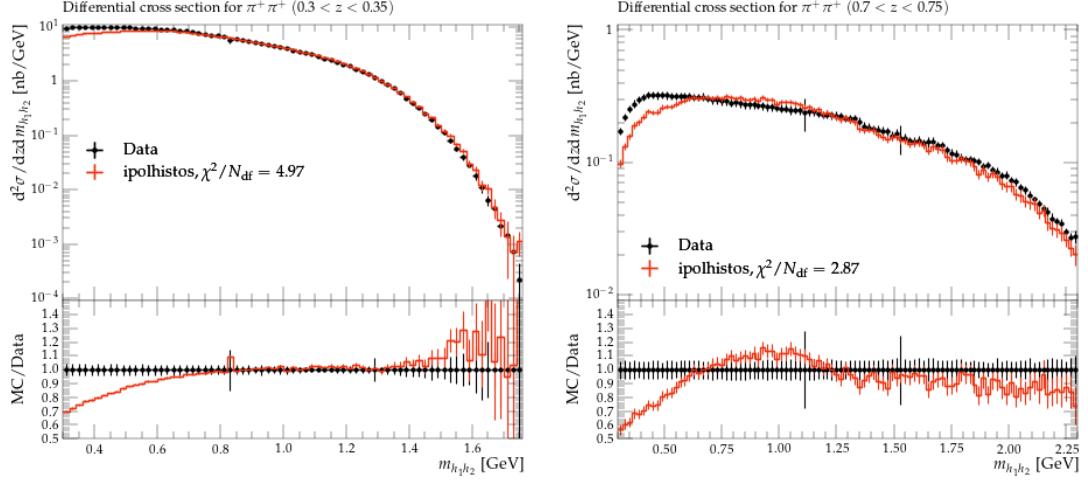


Figure 30: Left:  $\pi^+\pi^+$  pair cross sections as a function of the invariant mass  $m$  for the fractional energy bin  $0.3 - 0.35$ . Right: The same for the fractional energy bin  $0.7 - 0.75$ . The data is displayed by black points while the best fit result in red.

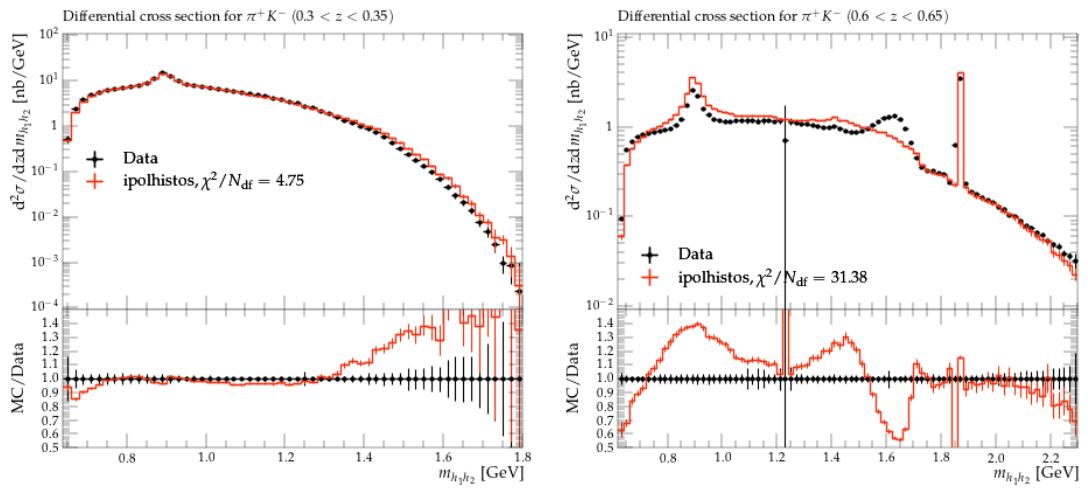


Figure 31: Left:  $\pi^+K^-$  pair cross sections as a function of the invariant mass  $m$  for the fractional energy bin  $0.3 - 0.35$ . Right: The same for the fractional energy bin  $0.6 - 0.65$ . The data is displayed by black points while the best fit result in red.

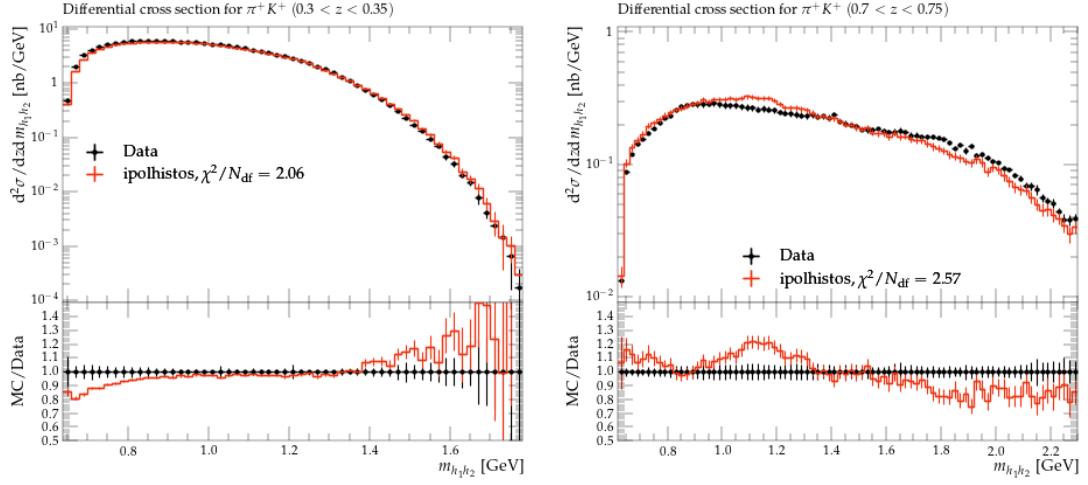


Figure 32: Left:  $\pi^+ K^+$  pair cross sections as a function of the invariant mass  $m$  for the fractional energy bin  $0.3 - 0.35$ . Right: The same for the fractional energy bin  $0.7 - 0.75$ . The data is displayed by black points while the best fit result in red.

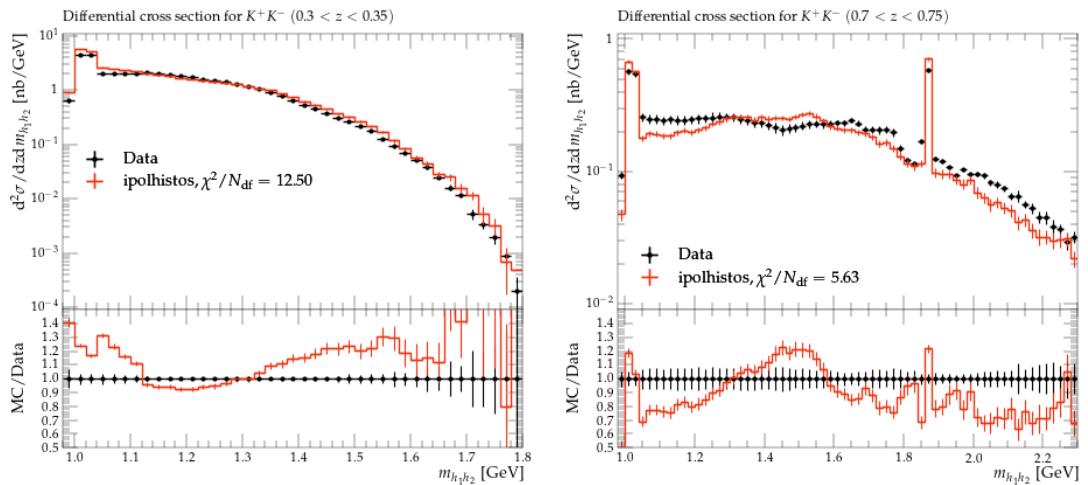


Figure 33: Left:  $K^+ K^-$  pair cross sections as a function of the invariant mass  $m$  for the fractional energy bin  $0.3 - 0.35$ . Right: The same for the fractional energy bin  $0.7 - 0.75$ . The data is displayed by black points while the best fit result in red.

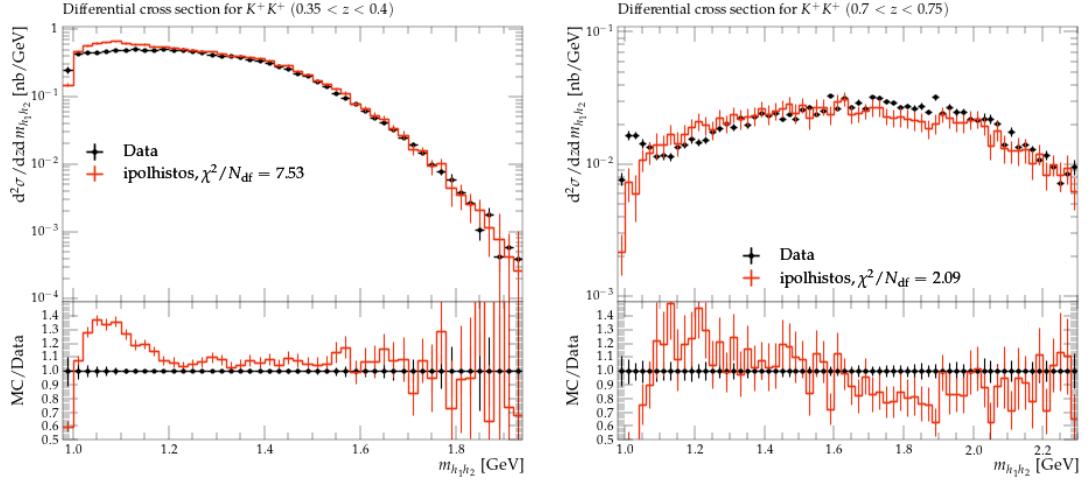


Figure 34: Left:  $K^+K^+$  pair cross sections as a function of the invariant mass  $m$  for the fractional energy bin  $0.35 < z < 0.4$ . Right: The same for the fractional energy bin  $0.7 < z < 0.75$ . The data is displayed by black points while the best fit result in red.

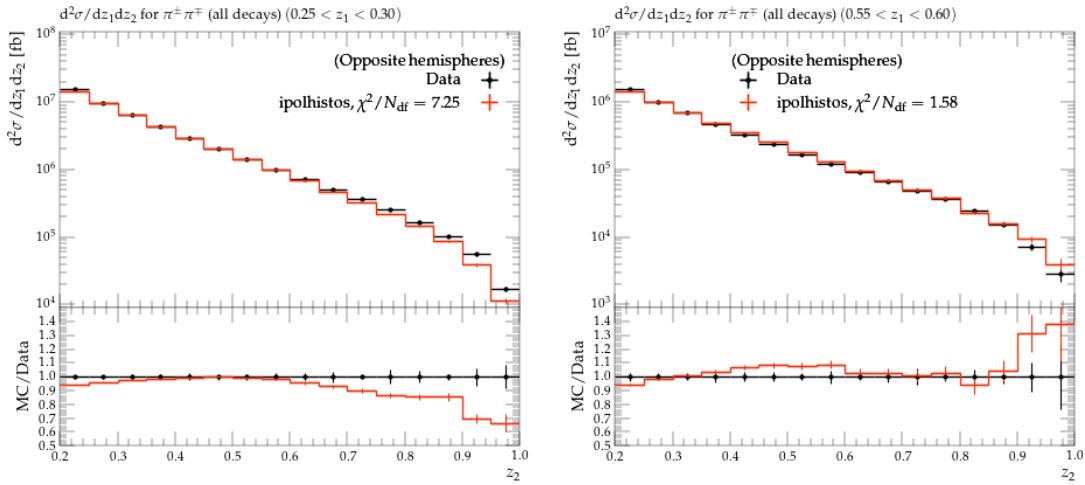


Figure 35: Left:  $\pi^+\pi^-$  pair cross sections in opposite hemispheres as a function of the invariant mass  $z_2$  for the fractional energy bin  $0.25 < z_1 < 0.3$ . Right: The same for the fractional energy bin  $0.55 < z_1 < 0.6$ . The data is displayed by black points while the best fit result in red.

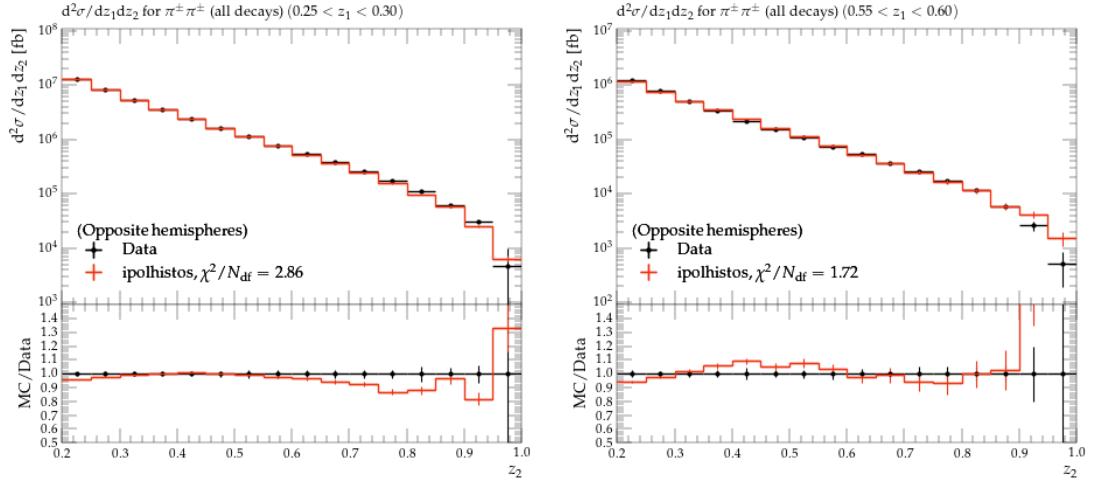


Figure 36: Left:  $\pi^+\pi^+$  pair cross sections in opposite hemispheres as a function of the invariant mass  $z_2$  for the fractional energy bin  $0.25 < z_1 < 0.3$ . Right: The same for the fractional energy bin  $0.55 < z_1 < 0.6$ . The data is displayed by black points while the best fit result in red.

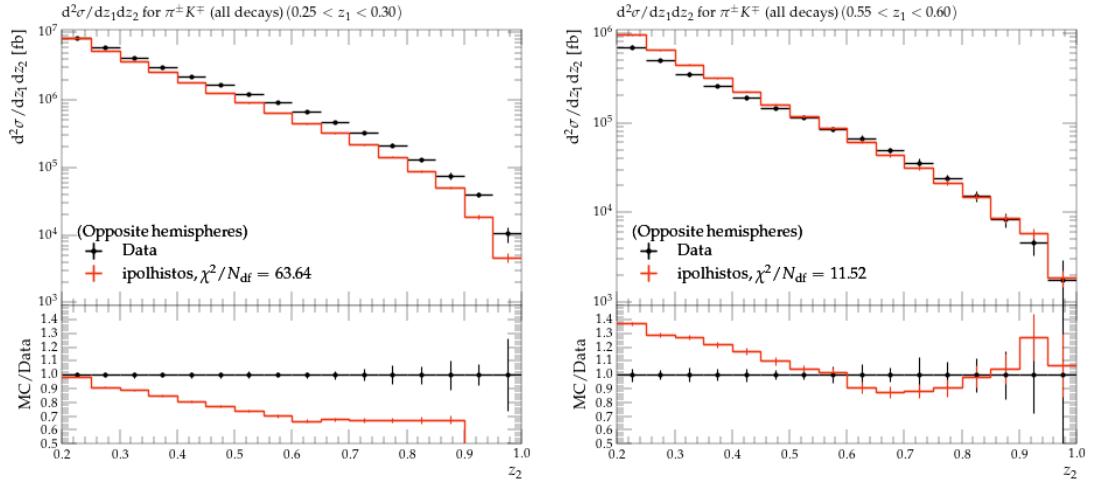


Figure 37: Left:  $\pi^+K^-$  pair cross sections in opposite hemispheres as a function of the invariant mass  $z_2$  for the fractional energy bin  $0.25 < z_1 < 0.3$ . Right: The same for the fractional energy bin  $0.55 < z_1 < 0.6$ . The data is displayed by black points while the best fit result in red.

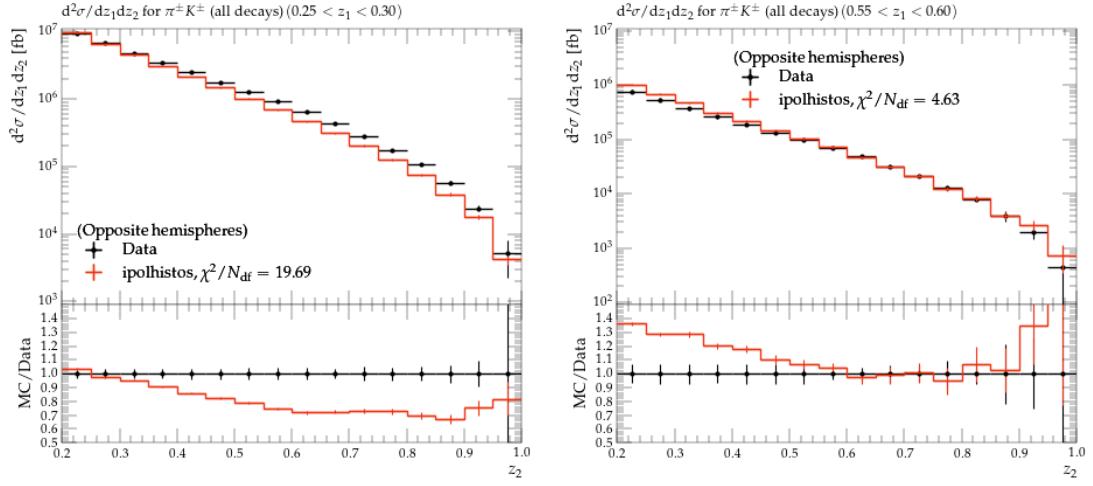


Figure 38: Left:  $\pi^+K^+$  pair cross sections in opposite hemispheres as a function of the invariant mass  $z_2$  for the fractional energy bin  $0.25 < z_1 < 0.3$ . Right: The same for the fractional energy bin  $0.55 < z_1 < 0.6$ . The data is displayed by black points while the best fit result in red.

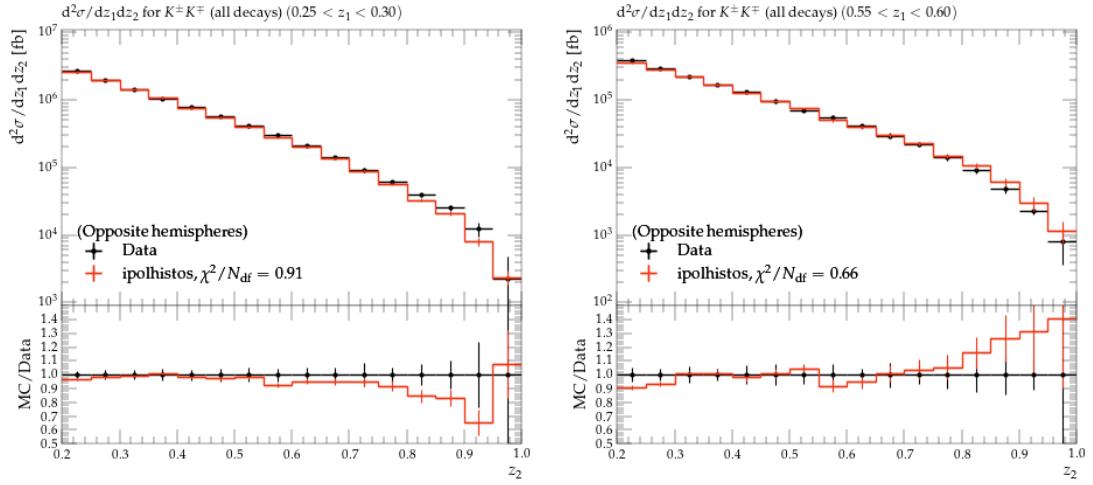


Figure 39: Left:  $K^+K^-$  pair cross sections in opposite hemispheres as a function of the invariant mass  $z_2$  for the fractional energy bin  $0.25 < z_1 < 0.3$ . Right: The same for the fractional energy bin  $0.55 < z_1 < 0.6$ . The data is displayed by black points while the best fit result in red.

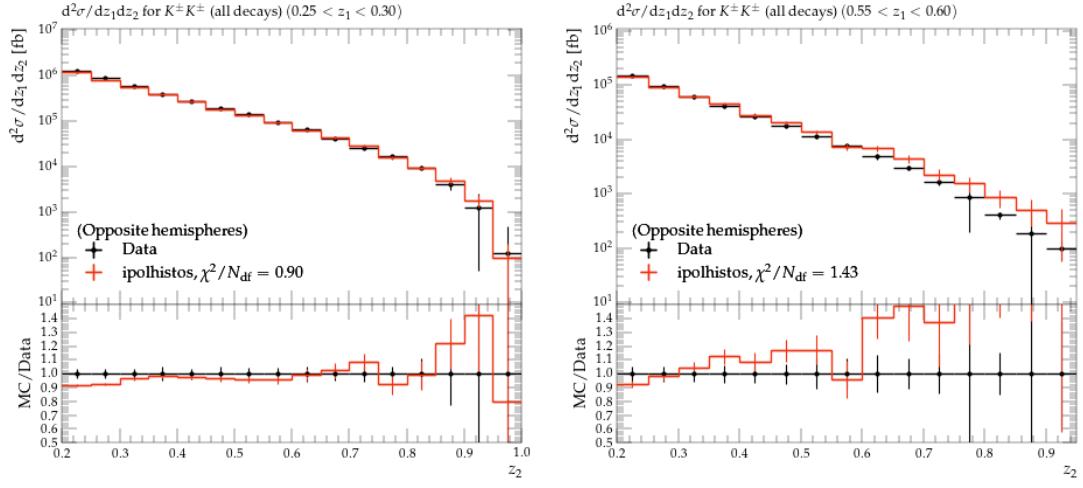


Figure 40: Left:  $K^+K^-$  pair cross sections in opposite hemispheres as a function of the invariant mass  $z_2$  for the fractional energy bin  $0.25 < z_1 < 0.3$ . Right: The same for the fractional energy bin  $0.55 < z_1 < 0.6$ . The data is displayed by black points while the best fit result in red.

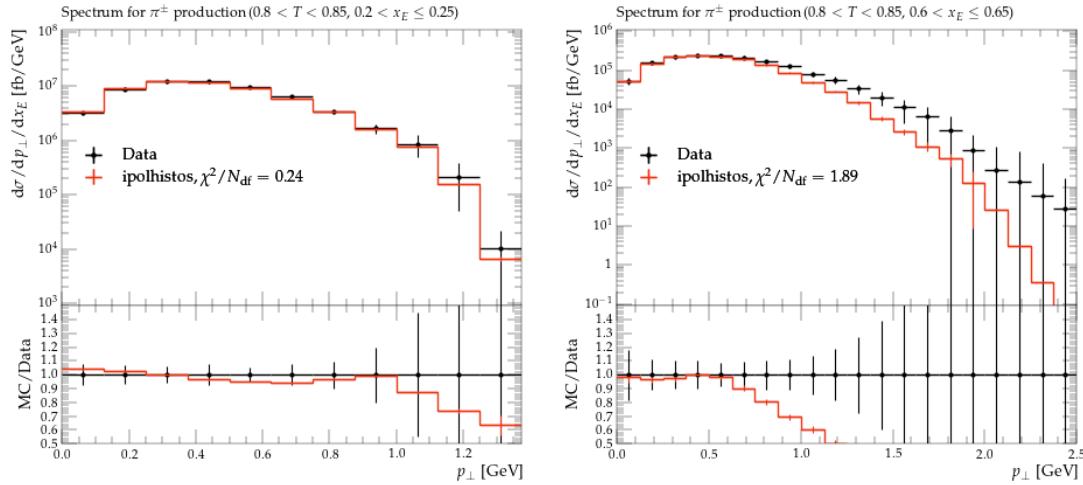


Figure 41: Left:  $\pi^\pm$  cross sections as a function of the transverse momentum  $p_T$  for the fractional energy bin  $0.2 < z_1 < 0.25$  in the thrust bin  $0.8 - 0.9$ . Right: The same for the fractional energy bin  $0.6 < z_1 < 0.65$ . The data is displayed by black points while the best fit result in red.

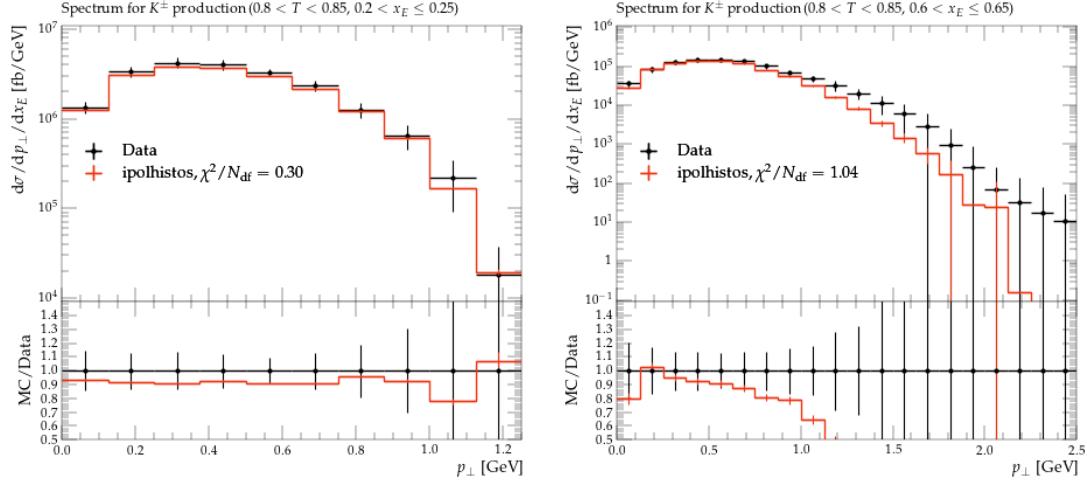


Figure 42: Left:  $K^\pm$  cross sections as a function of the transverse momentum  $p_T$  for the fractional energy bin  $0.2 < z_1 < 0.25$  in the thrust bin  $0.8 - 0.9$ . Right: The same for the fractional energy bin  $0.6 < z_1 < 0.65$ . The data is displayed by black points while the best fit result in red.

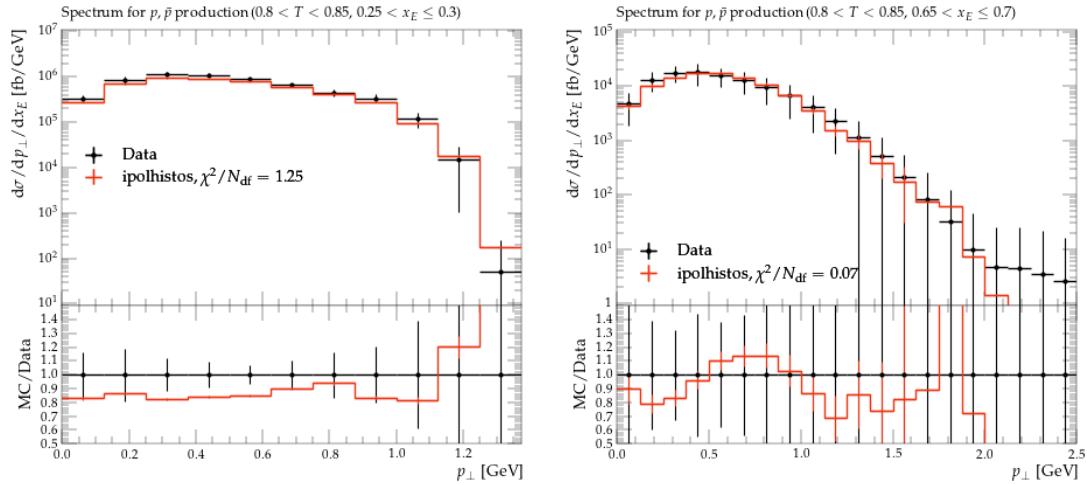


Figure 43: Left:  $p$  cross sections as a function of the transverse momentum  $p_T$  for the fractional energy bin  $0.2 < z_1 < 0.25$  in the thrust bin  $0.8 - 0.9$ . Right: The same for the fractional energy bin  $0.6 < z_1 < 0.65$ . The data is displayed by black points while the best fit result in red.

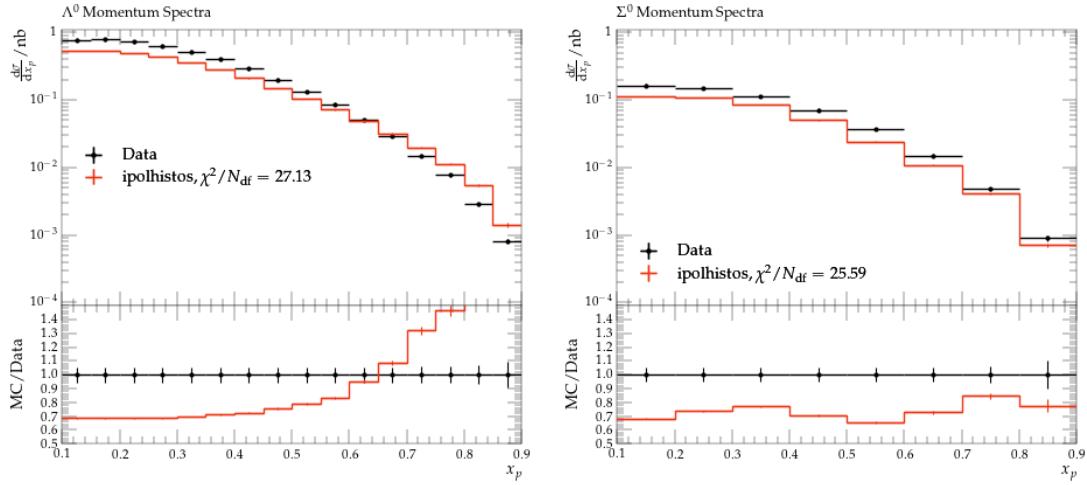


Figure 44: Left:  $\Lambda$  spectrum as a function of  $x_p$ . Right  $\Sigma^0$  spectrum as a function of  $x_p$ . The data is displayed by black points while the best fit result in red.

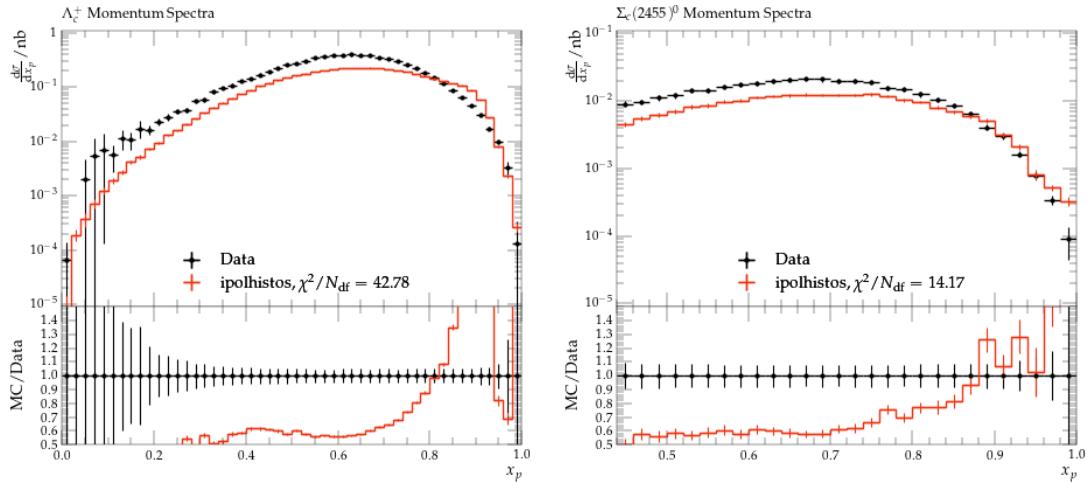


Figure 45: Left:  $\Lambda_c^+$  spectrum as a function of  $x_p$ . Right  $\Sigma_c(2455)^0$  spectrum as a function of  $x_p$ . The data is displayed by black points while the best fit result in red.

## 497 7.5 Hyperons and charmed baryons

498 For hyperons the description is still not as good, even after including the popcorn  
 499 variables and used the bug-fixed version of PYTHIA. The overall shapes do have  
 500 improved, however, as can be seen in Figs. 44 and 45 for some hyperons and charmed  
 501 baryons, respectively. The peak position of the charmed baryons is somewhat similar  
 502 to the measurements, but the tune predicts a rather abrupt drop-off of the cross  
 503 sections at very high momentum fractions that is not confirmed in the data, or at  
 504 least not as sharp.

## 505 8 Systematic uncertainties and tests

506 The best variables and their variations are summarized in Table 2 in comparison to  
 507 the default values of PYTHIA and currently in use in Belle2. In this table the best  
 508 values are given in the second column, the lower and upper values represent the  
 509 lowest and highest variations of the tune iterations to the best value (i.e. the last  
 510 iteration for that particular variable). The variations are just given as a measure  
 511 of how much these variables varied during the tuning evaluations and cannot be  
 512 considered as reliable uncertainties. In turn, the statistical uncertainties from the  
 513 tuning efforts are tiny and are therefore not tabulated. One can see that the variables  
 514 that have been retired after several iterations were quite stable. The corresponding  
 515 results are also highlighted in Fig. 46 in comparison to the other values.

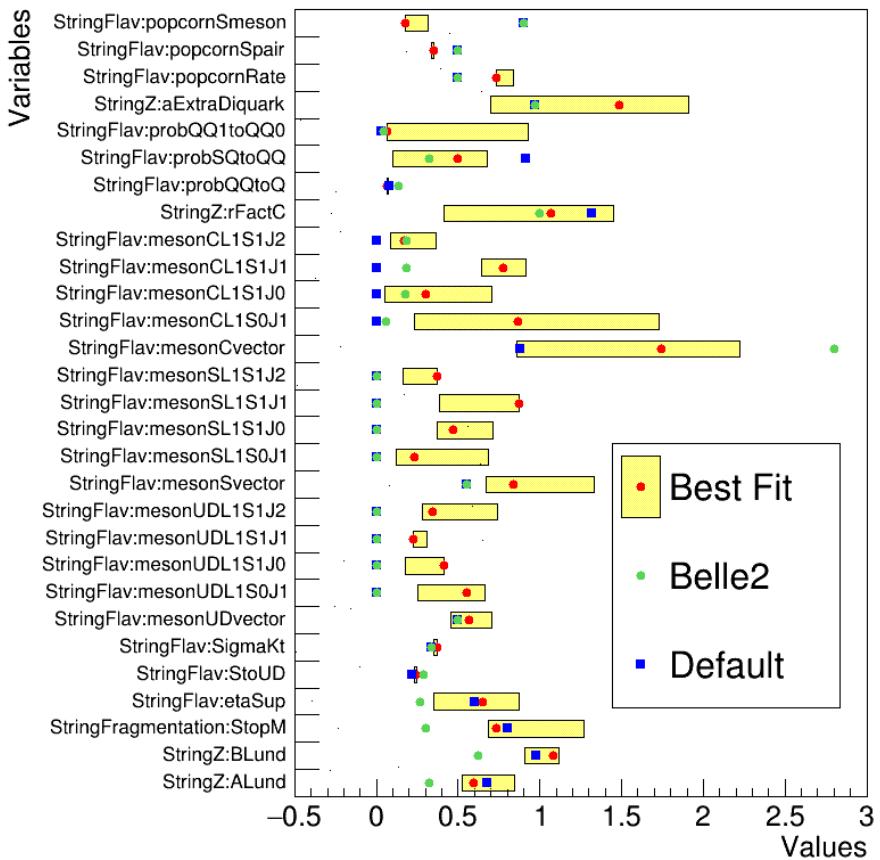


Figure 46: Best tune results (Red points), including their estimated uncertainties as discussed in the text (yellow bars) in comparison to the currently used (Darkgreen) and PYTHIA default (Blue boxes) values for each variable. Due to the significantly larger ranges, the results from mixing angles are not shown.,

516 The individual sets of variables and their variations are also visualized in the fol-  
 517 lowing figures as a function of their iterations. The Main Lund string fragmentation  
 518 variables can be found in Fig. 47. One sees again that the strangeness suppression  
 519 and the transverse momentum generation are indeed not changing much over the  
 520 iterations.

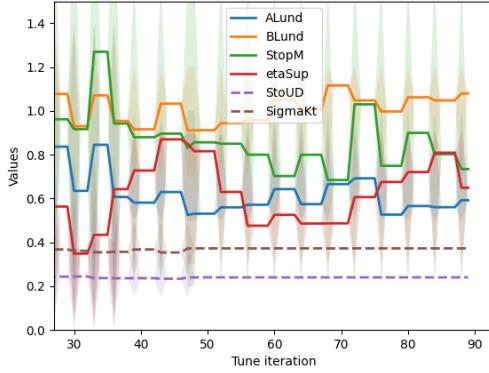


Figure 47: Main Lund variables, the allowed ranges are shown in shaded regions and the best values as a function of the various tuning iterations

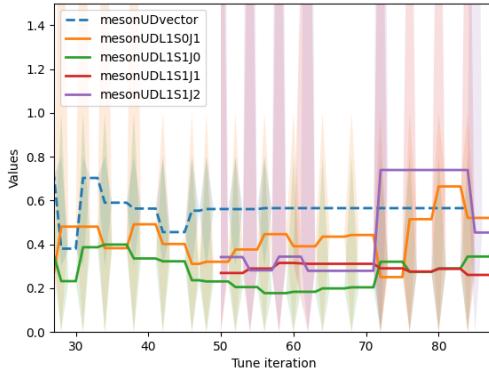


Figure 48: Light quark related vector meson and higher spin variables as a function of the various tuning iterations, the allowed ranges are shown in shaded regions and the best values as the center line. Dashed lines represent variables that have been fixed after they became stable.

521 The light quark vector meson and higher spin variables can be seen in Fig. 48.  
 522 Especially the higher spin variables are not particularly well determined and thus  
 523 fluctuate from iteration to iteration, but the vector meson fraction is fairly stable  
 524 which is why it was fixed eventually.

525 The corresponding strange and charm variables are displayed in Figs. 49 and 50,  
 526 respectively. In these, one can see that the two vector mesons fractions are again  
 527 the most stable variables and that the charm vector meson fraction is significantly  
 528 larger than that of strange quarks which again is slightly larger than that for light  
 529 quarks. The higher spin values typically vary much as well.

530 The baryon related fragmentation variables are displayed in Fig. 51. Apart from  
 531 the main diquark fragmentation and the extra Lund factor for diquarks, the values  
 532 are fluctuating significantly between iterations. After the inclusion of the popcorn  
 533 values, the vector diquark fraction also appears to stabilize.

534 The vector and pseudoscalar mixing angles are displayed in Fig. 52. Especially  
 535 the pseudoscalar mixing value is fluctuating significantly while the vector angle is

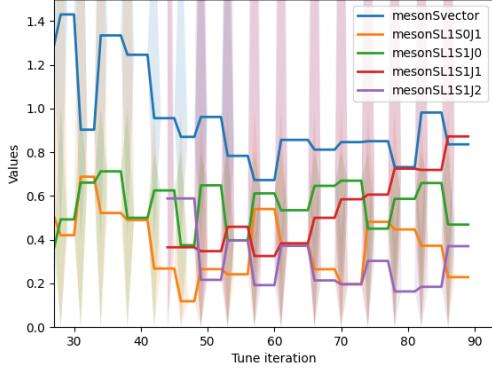


Figure 49: Strange quark related vector meson and higher spin variables as a function of the various tuning iterations, the allowed ranges are shown in shaded regions and the best values as the center line. Dashed lines represent variables that have been fixed after they became stable.

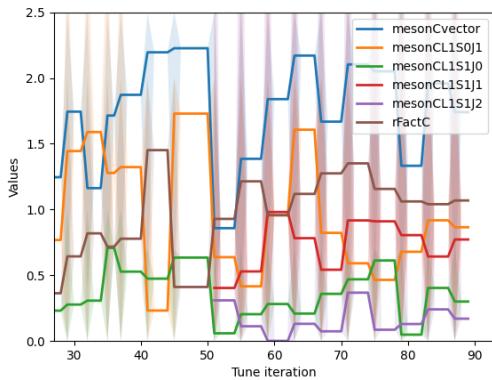


Figure 50: Charm quark related vector meson and higher spin variables as a function of the various tuning iterations, the allowed ranges are shown in shaded regions and the best values as the center line. Dashed lines represent variables that have been fixed after they became stable.

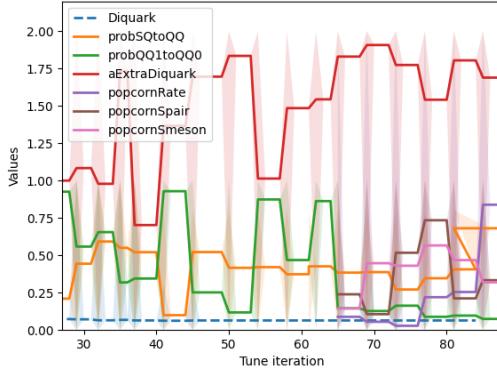


Figure 51: Baryon related variables as a function of the various tuning iterations, the allowed ranges are shown in shaded regions and the best values as the center line. Dashed lines represent variables that have been fixed after they became stable.

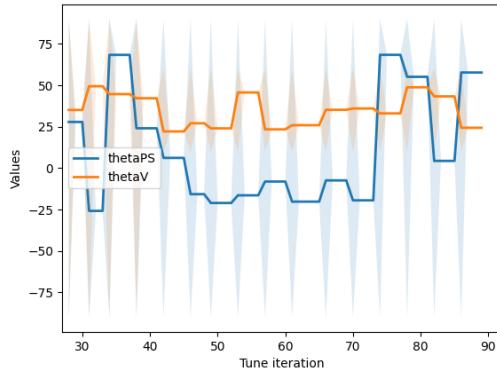


Figure 52: Mixing related variables as a function of the various tuning iterations, the allowed ranges are shown in shaded regions and the best values as the center line. Dashed lines represent variables that have been fixed after they became stable.

536 slightly more stable.

537 Last, the evolution of the goodness of fit as a function of the tune iterations is  
 538 displayed in Fig. 53. One can generally see that the reduced  $\chi^2$  did decrease for the  
 539 most part with the occasional fluctuations. After including the higher spin states  
 540 and fixing some variables not too much improvement can be seen. Another reduction  
 541 can be seen when including the popcorn variables at around tune iteration 65, but  
 542 again after an initial drop the values flatten out. The last improvement can be seen  
 543 from using the correct treatment of the extra  $a$  parameter that was fixed by the  
 544 PYTHIA maintainers from iteration 77. Since then, the  $\chi^2$  does not improve anymore  
 545 over two further iterations for each set of variables. This suggests that within the  
 546 space of variables, no significant further improvements can be achieved and likely  
 547 these are the best settings one can get.

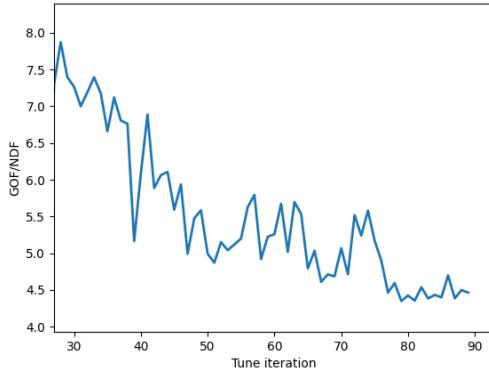


Figure 53: Evolution of the goodness of fit normalized by the number of degrees of freedom as a function of the various tuning iterations.

## 548 8.1 Comparison to older settings

549 It is also instructive to learn how the different settings after tuning compare to  
 550 the settings used as default or previously at Belle2. Those are displayed for vari-  
 551 ous measurements in the figures 54 to 61. Due to some empty bins in the latest  
 552 measurements which Rivet cannot handle well, the individual  $\chi^2/NDF$  for these  
 553 measurements are given as "nan". It is visible that while individual spectra for very  
 554 abundant particles such as light mesons are often reasonably well-described by the  
 555 older settings, especially di-hadron mass or momentum spectra and heavier particles  
 556 can be much better described after tuning.

557 Summing up all other  $\chi^2/NDF$  results gives average values of 15.3 for the Pythia  
 558 default settings, 14.4 for the previously used Belle2 settings and 6.3 for the latest  
 559 best settings. Note that these numbers are different from the actual fit numbers  
 560 since here the average over all individual spectra is taken, rather than summing all  
 561 points as is done in the fit. Those and the corresponding figures make it abundantly  
 562 clear, that the tuning effort successfully improved the description of the included  
 563 measurements.

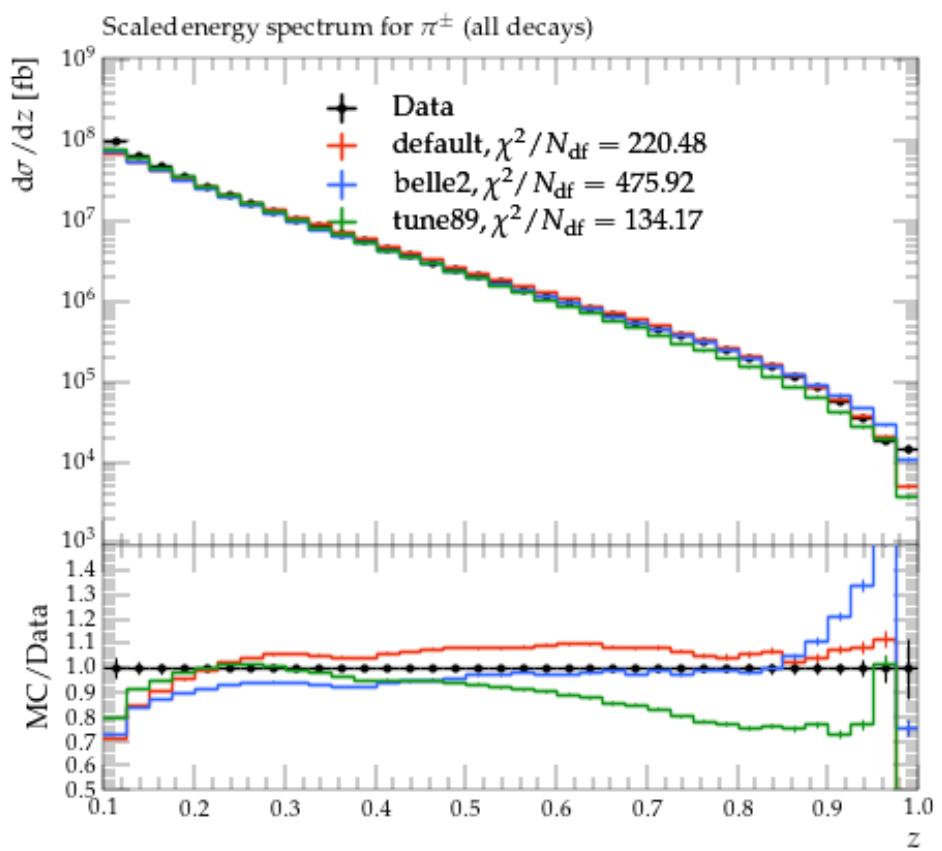


Figure 54: Pion cross sections as a function of the fractional energy  $z$ . The data is displayed by black points while the PYTHIA default is displayed in red, the current Belle2 setting in blue, and the best tune in green.

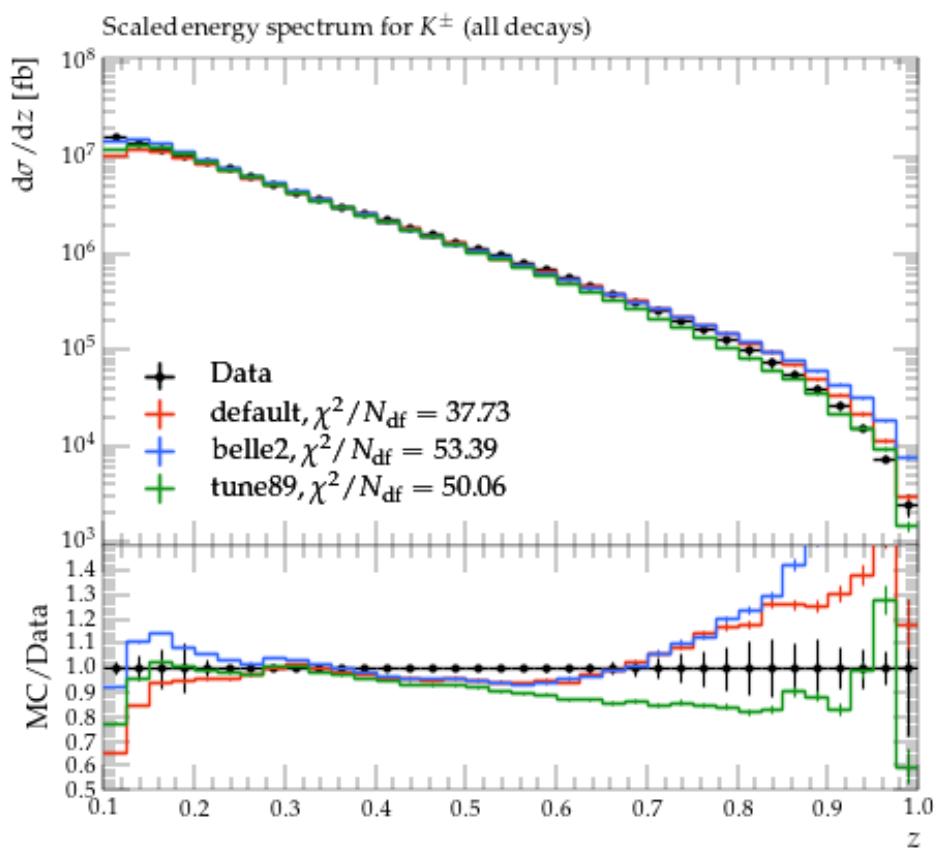


Figure 55: Kaon cross sections as a function of the fractional energy  $z$ . The data is displayed by black points while the PYTHIA default is displayed in red, the current Belle2 setting in blue, and the best tune in green.

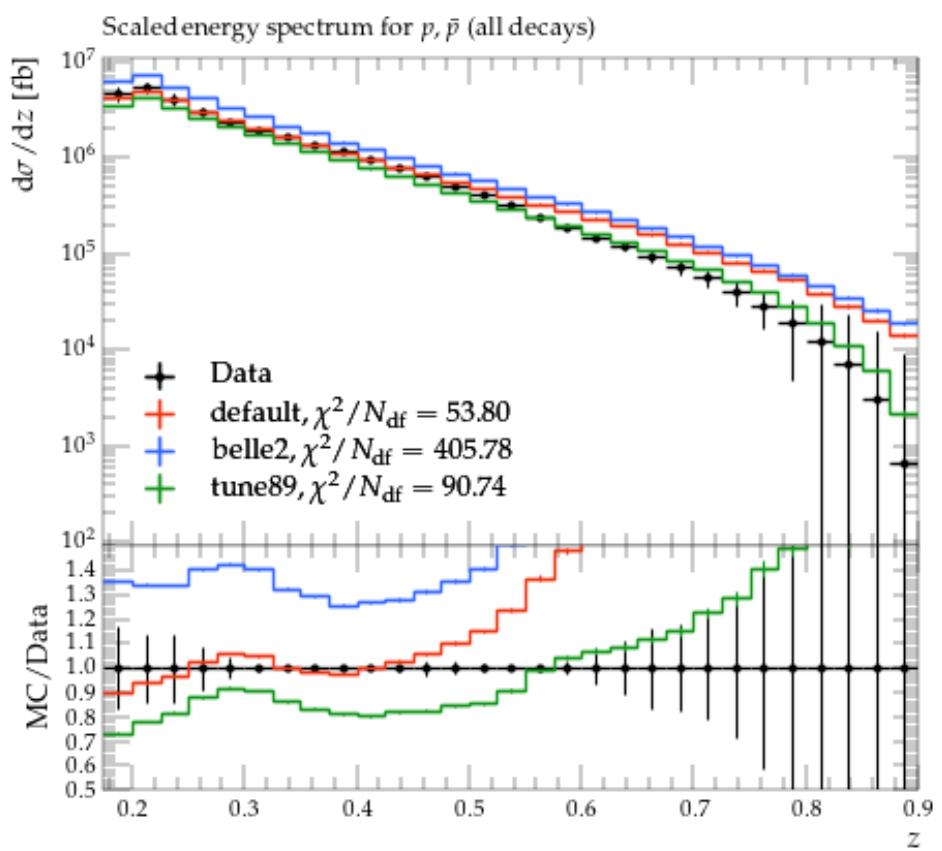


Figure 56: Proton cross sections as a function of the fractional energy  $z$ . The data is displayed by black points while the PYTHIA default is displayed in red, the current Belle2 setting in blue, and the best tune in green.

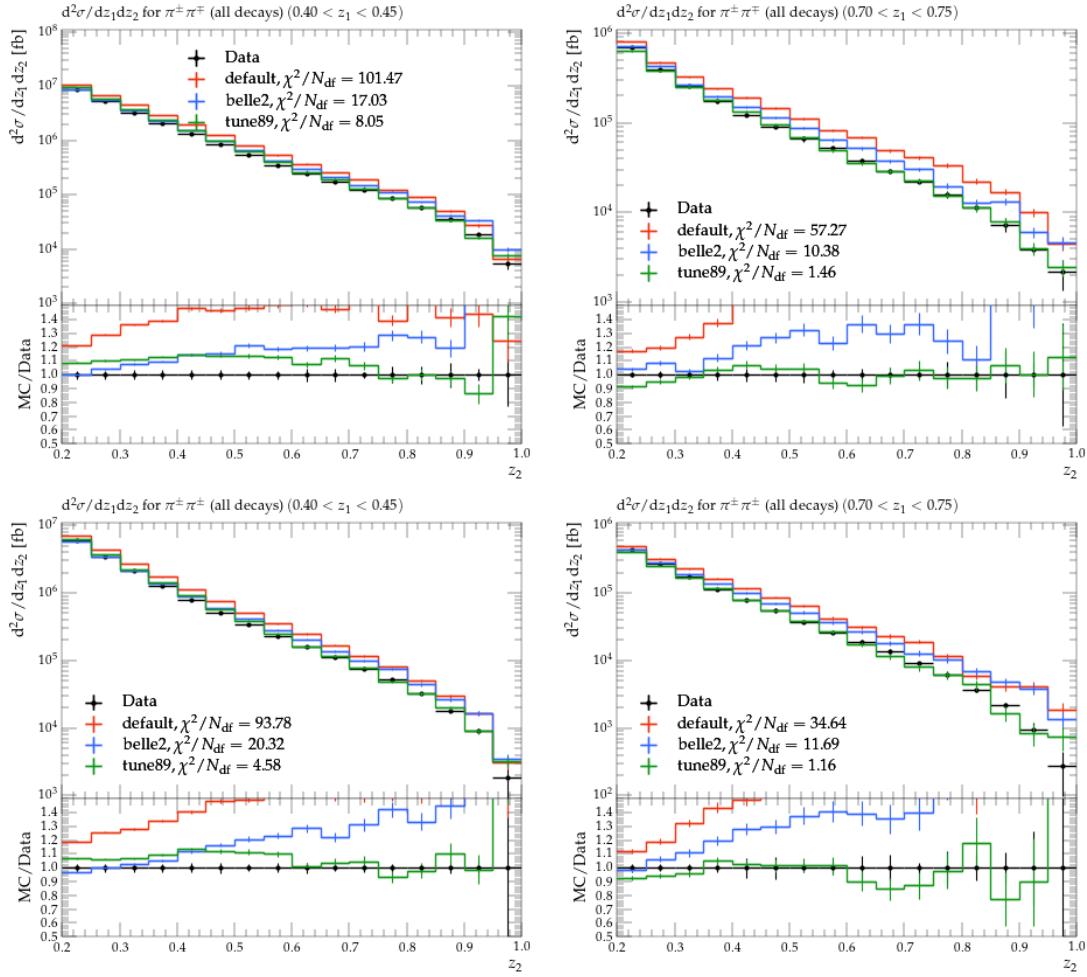


Figure 57: Top:  $\pi^\pm\pi^-$  spectra as a function of  $z_2$  for two bins of  $z_1$ . Bottom:  $\pi^\pm\pi^\pm$  spectra for the same  $z$  bins. The data is displayed by black points while the PYTHIA default is displayed in red, the current Belle2 setting in blue, and the best tune in green.

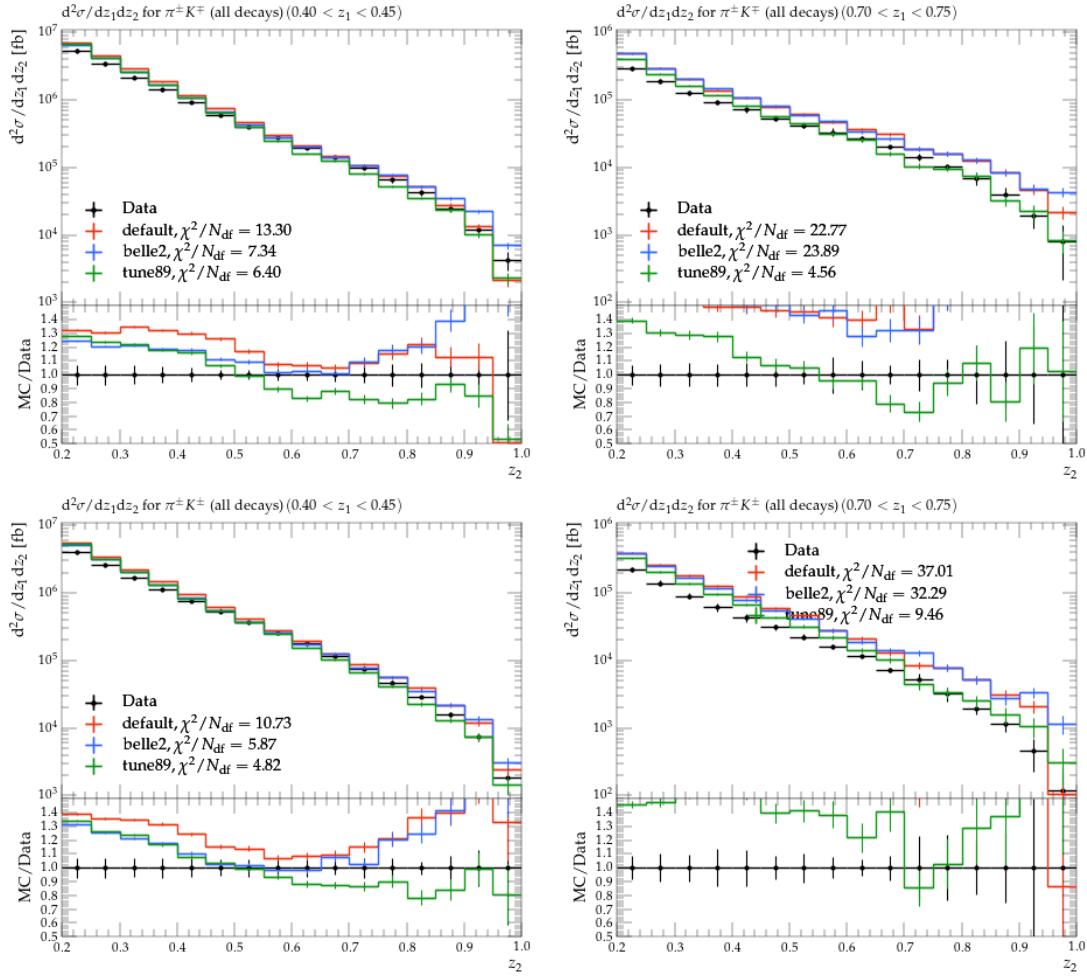


Figure 58: Top:  $\pi^+K^-$  spectra as a function of  $z_2$  for two bins of  $z_1$ . Bottom:  $\pi^\pm K^\pm$  spectra for the same  $z$  bins. The data is displayed by black points while the PYTHIA default is displayed in red, the current Belle2 setting in blue, and the best tune in green.

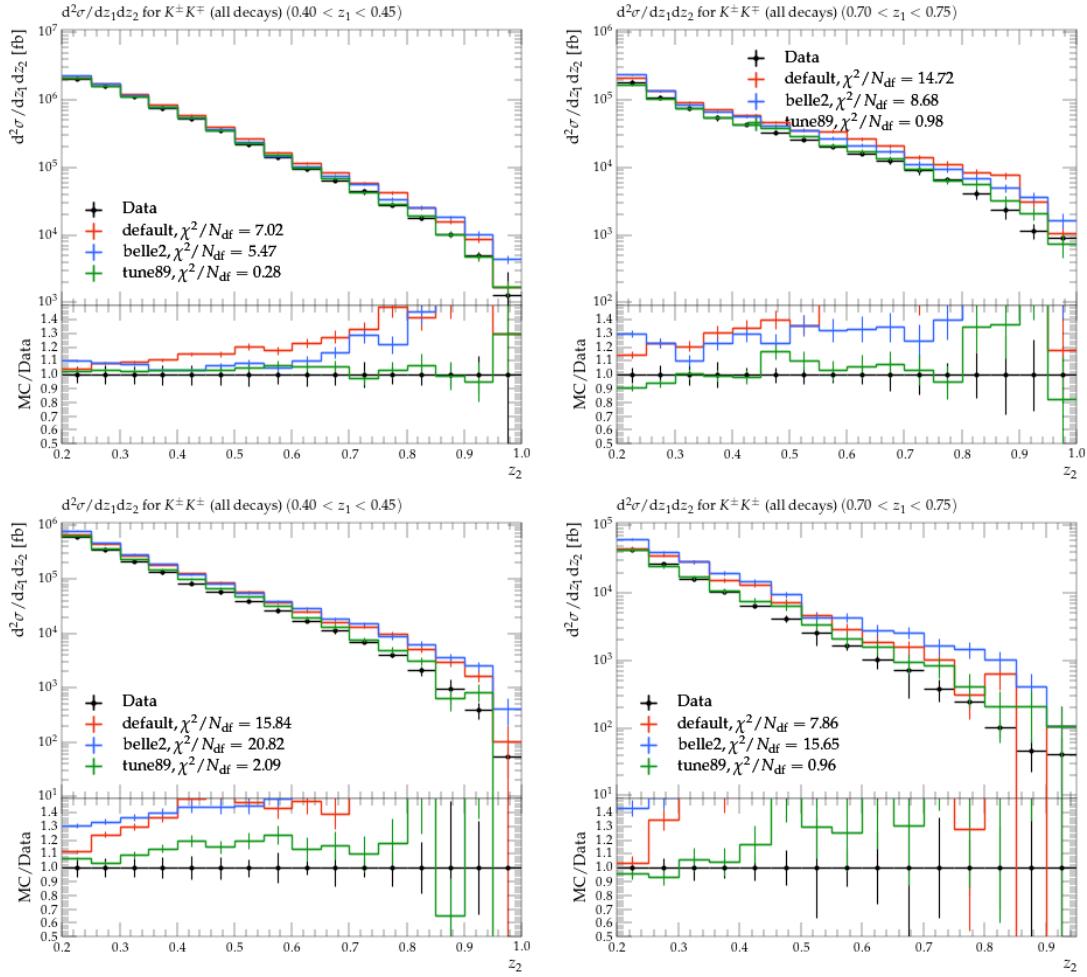


Figure 59: Top:  $K^+K^-$  spectra as a function of  $z_2$  for two bins of  $z_1$ . Bottom:  $K^\pm K^\pm$  spectra for the same  $z$  bins. The data is displayed by black points while the PYTHIA default is displayed in red, the current Belle2 setting in blue, and the best tune in green.

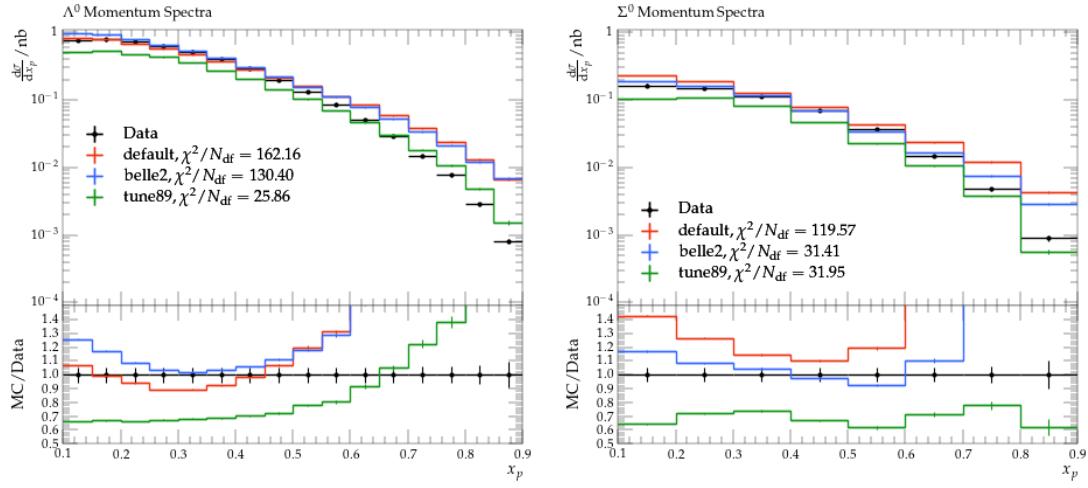


Figure 60: Left:  $\Lambda$  spectrum as a function of  $x_p$ . Right  $\Sigma^0$  spectrum as a function of  $x_p$ . The data is displayed by black points while the PYTHIA default is displayed in red, the current Belle2 setting in blue, and the best tune in green.

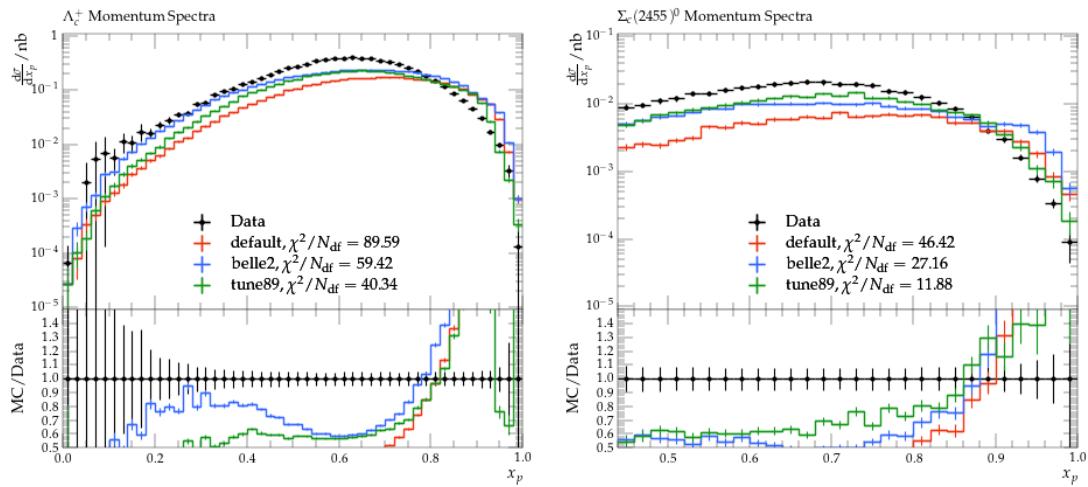


Figure 61: Left:  $\Lambda_c^+$  spectrum as a function of  $x_p$ . Right  $\Sigma_c(2455)^0$  spectrum as a function of  $x_p$ . The data is displayed by black points while the PYTHIA default is displayed in red, the current Belle2 setting in blue, and the best tune in green.

Table 2: Best tune variables and the variation of the best values during the various tune iterations as well as the PYTHIA default values and the current Belle2 values (release 8/9). Note, that Belle2 has also set the following values etaPrimeSub=0.12, MultIncrease=4.5, and MultIncreaseWeak=2.0 that were not studied here due to lack of sensitivity.

Variable	Best results	default	Belle2
StringZ:ALund	0.592 -0.067 +0.253	0.680	0.32
StringZ:BLund	1.080 -0.170 +0.036	0.980	0.62
StringFragmentation:StopM	0.734 -0.050 +0.535	0.800	0.3
StringFlav:etaSup	0.649 -0.301 +0.221	0.600	0.27
StringFlav:StoUD	0.240 -0.006 +0.004	0.217	0.286
StringFlav:SigmaKt	0.372 -0.019 +0.000	0.335	0.335
StringFlav:mesonUDvector	0.565 -0.109 +0.138	0.500	0.500
StringFlav:mesonUDL1S0J1	0.556 -0.306 +0.108	0	0
StringFlav:mesonUDL1S1J0	0.411 -0.234 +0.000	0	0
StringFlav:mesonUDL1S1J1	0.226 -0.000 +0.086	0	0
StringFlav:mesonUDL1S1J2	0.341 -0.061 +0.399	0	0
StringFlav:mesonSvector	0.836 -0.163 +0.498	0.550	0.550
StringFlav:mesonSL1S0J1	0.229 -0.110 +0.459	0	0
StringFlav:mesonSL1S1J0	0.469 -0.094 +0.243	0	0
StringFlav:mesonSL1S1J1	0.872 -0.489 +0.000	0	0
StringFlav:mesonSL1S1J2	0.370 -0.207 +0.001	0	0
StringFlav:mesonCvector	1.740 -0.882 +0.486	0.880	2.8
StringFlav:mesonCL1S0J1	0.865 -0.634 +0.864	0	0.06
StringFlav:mesonCL1S1J0	0.300 -0.252 +0.408	0	0.1775
StringFlav:mesonCL1S1J1	0.772 -0.129 +0.145	0	0.1868
StringFlav:mesonCL1S1J2	0.170 -0.084 +0.198	0	0.1836
StringZ:rFactC	1.069 -0.658 +0.383	1.32	1.0
StringFlav:probQQtoQ	0.064 -0.002 +0.008	0.081	0.133
StringFlav:probSQtoQQ	0.497 -0.398 +0.184	0.915	0.323
StringFlav:probQQ1toQQ0	0.065 -0.000 +0.864	0.0275	0.0468
StringZ:aExtraDiquark	1.487 -0.785 +0.420	0.970	0.970
StringFlav:popcornRate	0.734 -0.000 +0.104	0.500	0.500
StringFlav:popcornSpair	0.350 -0.016 +0.000	0.500	0.500
StringFlav:popcornSmeson	0.180 -0.000 +0.139	0.900	0.900
StringFlav:thetaPS	57.719 -78.753 +10.675	-15.	-15.
StringFlav:thetaV	24.353 -0.952 +24.444	26.	26.

## 564 9 Results

565 The best results of the tuning exercise are already tabulated in table 1 together with  
566 the default values used in PYTHIA8.3 and BelleII. The overall confidence in the best  
567 results is high as indicated by the data-tune comparisons in the previous chapters.  
568 There are however different levels of how confident the best variables are depending  
569 on the overall sensitivities. Based on those, the main Lund parameters are probably  
570 very well determined by the tuning as the sensitivities are very high. The vector me-  
571 son related variables are also fairly well determined thanks to the latest Belle paper  
572 [3] which explicitly looked at the fragmentation of vector mesons. The higher spin  
573 related variables are somewhat less determined due to the fact that no explicit mea-  
574 surements of these particles are available. There is some indirect sensitivity via the  
575 invariant mass distributions where the higher mass ranges get populated from such  
576 particle decays. Last, the baryon related variables seem to be also well-determined,  
577 but it is obvious by the differences from the tune to the data that the description of  
578 baryon fragmentation in the Lund model seems to be still lacking. It will be still bet-  
579 ter to use the optimized values, but there need to be also significant improvements  
580 on the model description itself to really obtain a very reliable description of bary-  
581 onic final states. As a next step for the BelleII continuum simulation development,  
582 it will be important to see whether the optimized settings also directly translate into  
583 significant improvements within the overall BelleII simulation framework that uses  
584 EvtGen for decays rather than the standalone PYTHIA used in these studies.

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## 610 A Pythia StringZ:aExtraDiquark bugfix related 611 changes

612 As indicated in communication by the PYTHIA team, a bug was found in their port-  
613 ing of the String fragmentation routines from fortran-based sc pythia6 to PYTHIA8  
614 which persisted until version 8.3.14. This bug was related to the handling of the  
615 variable StringZ:aExtraDiquark. This behavior was fixed in later versions, but since  
616 most tuning efforts using older versions obtained best parameters that included this  
617 bug, a switch was introduced to still use the old, incorrect treatment or the corrected  
618 one by: StringZ:useOldAExtra = on/off. To test the actual behavior on the Belle2  
619 tuning efforts, the best tune iteration at that time (tune71) was compared for the  
620 old, previously used PYTHIA version 8.3.13, and the latest version 8.3.16 either hav-  
621 ing the old or new treatment explicitly switched on or off. As expected, these changes  
622 had no visible effect on any of the meson related measurements used in the tune op-  
623 timization. When using the old treatment, also no sizable changes were observed for  
624 the various baryon measurements, but the behavior between old and new treatment  
625 was significantly different. As intended for this variable, the high- $z$  or  $x_p$  shapes be-  
626 came softer with the new treatment which resulted in a generally better description  
627 of the proton cross sections. Also the behavior of hyperon and charmed baryon cross  
628 sections visibly improved while the overall magnitudes are still not well described.  
629 The corresponding comparisons are shown in Figs. 62 and 63 for protons, several  
630 hyperons and charmed baryons. In these comparisons, it is also visible that the de-  
631 fault behavior (i.e. without explicitly setting the StringZ:useOldAExtra = on/off  
632 variable) corresponds to the old setting. Because of these changes, and the improve-  
633 ments that go with them, the remainder of the tuning effort was performed using  
634 the PYTHIA version 8.3.16 and using the new treatment via StringZ:useOldAExtra  
635 = off.

636 Initially, it was not clear, that the old treatment is still used per default, which re-  
637 sulted in the first tuning efforts after this switch to still use it. Only from tune76 for-  
638 ward the new, correct treatment was explicitly implemented via StringZ:useOldAExtra  
639 = off.

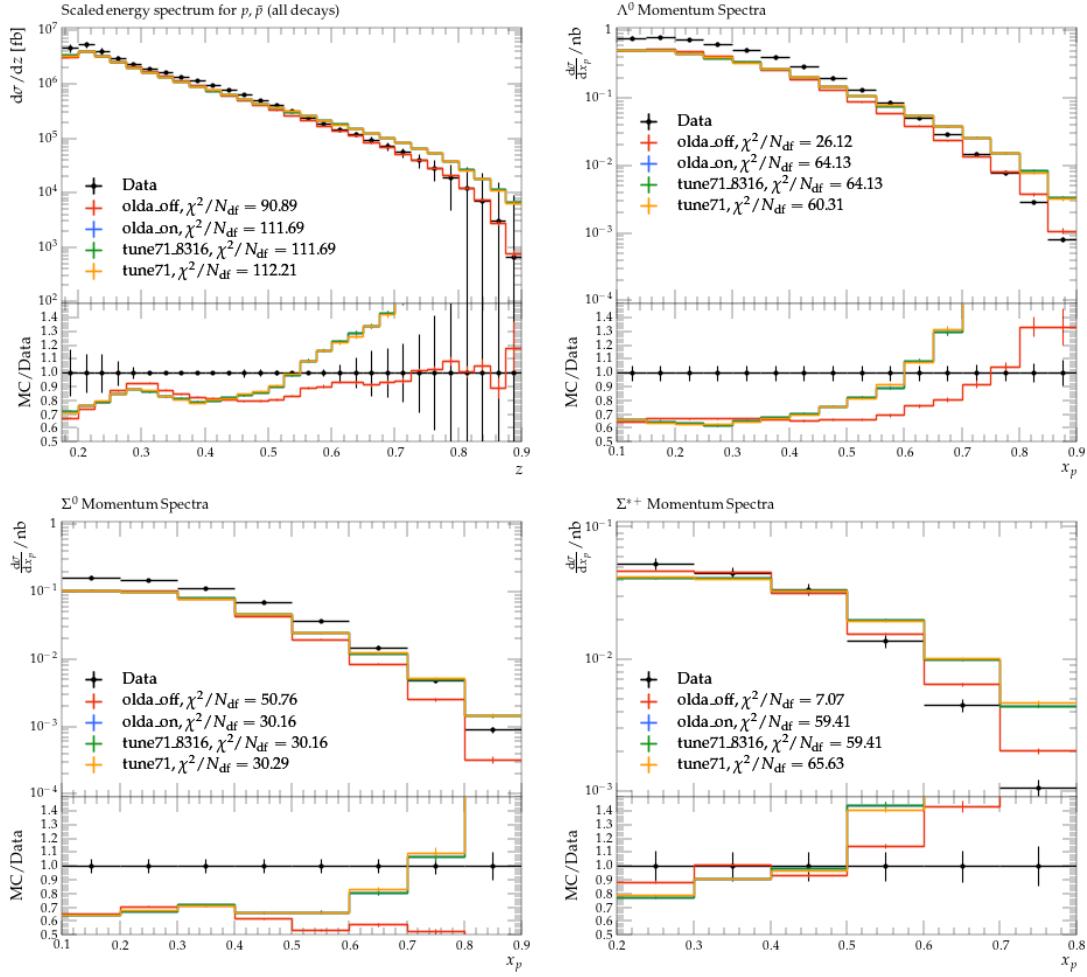


Figure 62: Comparison of the distributions for protons (top left),  $\Lambda$  (top right),  $\Sigma^0$  (bottom left) and  $\Sigma^{*+}$  as a function of energy or momentum fraction. The black points correspond to the measurements while the yellow points correspond to the best values after tune 71 using PYTHIA8.3.13, the green points correspond to the same tune but using PYTHIA8.3.16, the blue points use the same but explicitly setting `StringZ:useOldAExtra` to "on", and the red points correspond to the same, but switching it to "off".

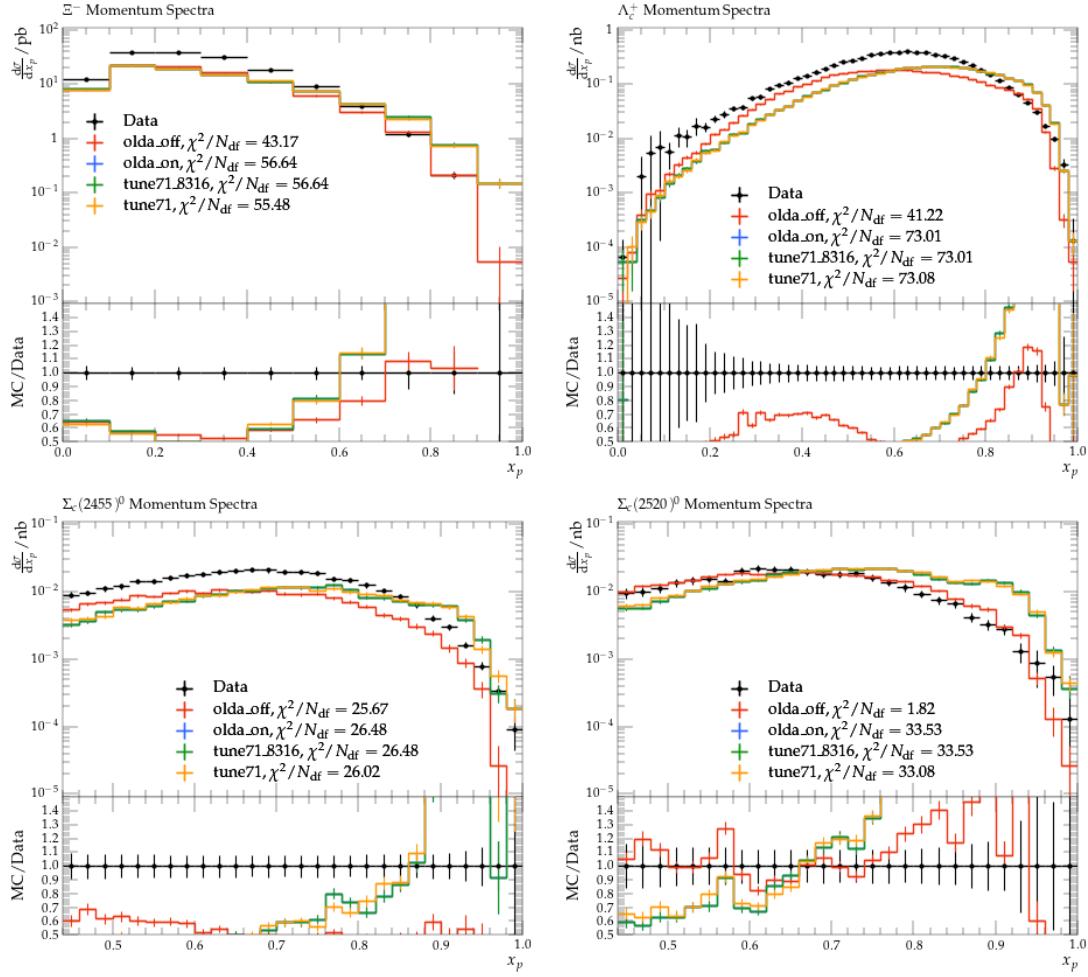


Figure 63: Comparison of the distributions for  $\Xi^-$  (top left),  $\Lambda_c$  (top right),  $\Sigma_c^0(2455)$  (bottom left) and  $\Sigma_c^0(2520)$  as a function of momentum fraction. The black points correspond to the measurements while the yellow points correspond to the best values after tune 71 using PYTHIA8.3.13, the green points correspond to the same tune but using PYTHIA8.3.16, the blue points use the same but explicitly setting `StringZ:useOldAExtra` to "on", and the red points correspond to the same, but switching it to "off".