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RapidSim: an application for the fast simulation of heavy-quark hadron decays

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Abstract

RapidSim is a lightweight application for the fast simulation of phase space decays of beauty and charm quark hadrons, allowing for quick studies of the properties of signal and background decays in particle physics analyses. Based upon the `TGenPhaseSpace` class from the ROOT application it uses externally provided fixed-order next-to-leading-logarithm calculations to boost the initial beauty and charm hadrons to the appropriate energy for the production environment of interest. User-defined momentum resolution functions can be used to mimic the effect of imperfect track reconstruction. User-defined efficiency shapes can be applied during generation to reproduce the effects of geometric and kinematic requirements on final state particles as well as the dynamics of the decay. The effect of mis-identification of the final state particles is simple to configure via configuration files, while the framework can easily be extended to include additional particle types. This paper describes the RapidSim framework, features and some example use cases.

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1 Introduction

A common problem in the analysis of particle decays is understanding the kinematic properties of the signal decay of interest and the potential backgrounds that can be introduced via other particle decays that have been imperfectly reconstructed in the detector. In particular, it is often crucial to know the shape of the invariant mass of the final state particles (or sub-sets of them) and the corresponding shape of the background decays. These backgrounds can arise from a number of sources:

- Decays to final states containing a sub-set of the particles in the signal decay;

- Decays to final states containing the same particles as in the signal decay, with additional particles that have not been reconstructed by the detector;

- Decays to final states where some of the particles have been misidentified by the detector such that they appear as the signal decay;

- Some combination of the above.

One method to study potential background sources is to generate large samples of the decays and pass them through the full detector simulation and reconstruction software chain. By selecting these events as if they are the signal decay, it is possible to study the shape of the backgrounds in the invariant mass distribution of interest. The disadvantage of this approach is the typically long time required to generate, reconstruct and select these background samples and the mass storage requirements to retain these samples.

RapidSim [1] is an application that allows analysts to quickly generate large samples (a few seconds for millions of events) of potential background decays with momentum spectra, invariant mass resolutions and efficiency shapes that are close approximations to what can be obtained from a full detector simulation. The speed of generation allows analysts to quickly perform initial studies that may indicate avenues for further investigation that may need a more detailed simulation. RapidSim supports the generation of a single decay chain with any number of sub-decays. It utilises the ROOT [2] software package and, specifically, the `TGenPhaseSpace` class to perform the fast generation. Fixed-order next-to leading-log (FONLL) [3] calculations are used to provide the correct kinematic properties of the heavy hadrons. By default, RapidSim is deployed with appropriate FONLL configuration files such that heavy hadrons are produced with the kinematic properties that are expected from proton-proton collisions at the CERN Large Hadron Collider [4]. In addition to generating decays in 4π it is possible for the user to specify that the decays of interest fall within the geometrical acceptance of the LHCb experiment [5]. The simple design allows users to extend RapidSim to include alternative detector geometries. RapidSim can accommodate basic user-defined kinematic efficiency effects during generation and mis-identification of final-state particles. All of these features are implemented in a generic way to enable them to be configured for any decay chain.

Section 2 of this paper describes how to compile and run the application. Sections 3 and 4 give an overview of the configuration options and example use case, respectively. Details of the heavy quark production, efficiency effects, track momentum resolution and

particle mis-identification can be found in Sections 5, 6, 7 and 8, respectively. A summary is presented in Section 9.

2   Usage

The latest version of the source code can be found on GitHub [1] and is compiled using the following commands:

```
mkdir build
cd build
cmake ..
make
```

The user should define the environment variable `RAPIDSIM_ROOT` to point to the root of the `RapidSim` directory structure. The executable may then be run as

```
$RAPIDSIM_ROOT/build/src/RapidSim.exe <decay mode> <events to generate> [<save tree?>]
```

for example,

```
$RAPIDSIM_ROOT/build/src/RapidSim.exe Bs2Jpsiphi 10000 1
```

where there is a user provided `Bs2Jpsiphi.decay` file and optionally a user-defined `Bs2Jpsiphi.config` file (described in Sections 3 and 4) in the present working directory.

3   Configuration

The RapidSim package has been designed to be easily configurable at run time for any decay, with all options relating to the decay configured via a decay-specific configuration file. This file is automatically created, with default options, the first occasion a particular decay is generated. Full lists of the available global and particle-specific settings are given in Tables 1 and 2, respectively. For most settings, the syntax is `<setting> : <option>`, where spaces and/or commas may be used to separate multiple options. The `param`, `shape` and `cut` global settings require multiple arguments to be provided, with the following syntax:

```
param : <name> <type> <particles> [TRUE]
shape : <file> <hist> <paramX> [<paramY>]
cut : <param> <type> <value1> [<value2>]
```

For `param`, `<type>` is one of the parameter types defined in Table 3, `<particles>` is a space separated list of particles to combine to calculate the parameter and the optional `TRUE` defines the parameter in terms of true four-momenta rather than reconstructed quantities. For `shape`, `<file>` and `<hist>` must give the filesystem location and name of a TH1 or TH2 object, and the `<param{X,Y}>` fields must match the `<name>` field of defined parameters. For `cut`, `<param>` must match the name of a defined parameter, `<type>` must be one of `min`, `max`, `range` or `veto`, and `<value1>` and `<value2>` define the cutoff values.

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Table 1: Global settings configured via the decay configuration file.

Setting	Description	Options (default)
seed	sets the seed for the random number generator	integer values (4357)
acceptance	sets the type of geometric acceptance to apply to the decay	(Any), ParentIn, AllIn AllDownstream
energy	sets the pp collision energy (in TeV) used to get the correct parent kinematics	7, (8), 13, 14
parent	overrides the determined flavour of the parent particle used to get the correct parent kinematics	(b), c * default is c for decays of charmed hadrons
geometry	sets the detector geometry to use for production and acceptance	4pi, (LHCb)
ptRange	sets the range of p_T to generate the parent within	two float values (0 100)
etaRange	sets the range of η to generate the parent within	two float values (1 6)
minWidth	sets the minimum resonance width (in GeV) to be generated. Narrower resonances will be generated with a fixed mass.	float values (0.001)
maxAttempts	sets the maximum number of attempts allowed to generate each decay.	integer values (1000)
paramsStable	Defines the set of parameters to be added to the histograms/tree for each stable particle in the decay.	(P, PT), M, M2, MT, E, ET, PX, PY, PZ, eta, phi, rapidity, gamma, beta
paramsDecaying	Defines the set of parameters to be added to the histograms/tree for each decaying particle in the decay.	(P, PT, M), M2, MT, E, ET, PX, PY, PZ, eta, phi, rapidity, gamma, beta
paramsTwoBody	Defines the set of parameters to be added to the histograms/tree for each two-body combination of particles in a 3+-body decay.	P, PT, M, (M2), MT, E, ET, PX, PY, PZ, eta, phi, rapidity, gamma, beta
paramsThreeBody	Defines the set of parameters to be added to the histograms/tree for each three-body combination of particles in a 4+-body decay.	P, PT, M, (M2), MT, E, ET, PX, PY, PZ, eta, phi, rapidity, gamma, beta
param	Defines a new parameter to be added to the histograms/tree.	See text for details
cut	Applys a cut on a given parameter.	
shape	Sets a 1D or 2D PDF to generate events according to.	

Table 2: Particle settings configured via the decay configuration file.

Setting	Description	Options (default)
name	A user-friendly name for this particle to be used in variable names.	alphanumeric
smear	The type of momentum smearing to apply to this particle.	types of smearing (LHCb-Generic) * defaults to LHCb-Electron for $e^{\pm}$.
invisible	Whether the particle should be treated as invisible. Invisible particles are not included when determining non-truth parameters. A corrected mass parameter will be added automatically if any particles are invisible.	true, (false) * defaults to true for neutrinos.
altMass	Adds alternative mass hypotheses for this particle.	particle type names

Table 3: Types of parameter and their corresponding descriptions.

Type	Description
M	The invariant mass of the combination of the given particles
M2	The squared invariant mass of the combination of the given particles
MT	The transverse mass of the combination of the given particles
E	The energy of the combination of the given particles
ET	The transverse energy of the combination of the given particles
P	The total momentum of the combination of the given particles
PX	The X momentum of the combination of the given particles
PY	The Y momentum of the combination of the given particles
PZ	The Z momentum of the combination of the given particles
PT	The transverse momentum of the combination of the given particles
eta	The pseudorapidity of the combination
phi	The azimuthal angle of the combination
y	The rapidity of the combination
gamma	The relitivistic gamma factor of the combination
beta	The velocity of the combination
theta	The angle between the first two particles in the rest frame of the combination of the remaining particles *e.g.* "1 2 1 3" would give the angle between 1 and 2 in the rest frame of a resonance in m_{13}
costheta	The cosine of theta
Mcorr	The corrected mass of the combination of the given particles correcting for any invisible particles. Given by $m_{\mathrm{corr}} = \sqrt{m^2 + p_{\mathrm{T}}^{\mathrm{miss}\,2}} + p_{\mathrm{T}}^{\mathrm{miss}}$, where m is the reconstructed mass and $p_{\mathrm{T}}^{\mathrm{miss}}$ is the momentum of the reconstructed particles transverse to the true flight direction of the combination of all given particles.

In addition to the decay-specific configuration file. Several common configuration files are located in the `config/` and `rootfiles/` directories such as

- the list of defined particle species;

- definitions of production kinematics options;

- definitions of momentum resolution options.

Further details on the configuration of these latter two features are given in Sections 5.1 and 7.1, respectively.

4   Example: $B_s^0 \rightarrow J/\psi\,\phi$

The decay file consists of a single line, which describes the decay using the following syntax:

- particles are named according to `config/particles.dat` and separated by spaces;

- a decay is denoted by `->`;

- subdecays are demarcated by braces {}.

For the $B_s^0 \rightarrow J/\psi\,\phi$ decay the `Bs2Jpsiphi.decay` ASCII file contains the single line

```
Bs0 -> { Jpsi -> mu+ mu- } { phi -> K+ K- }
```

where the particle names are defined in the `config/particle.dat` file. In this example the J/ψ (ϕ) meson decays to two oppositely charged muons (kaons). The user-defined configuration file (auto-produced the first time a particular decay is generated) is written as:

```
paramsDecaying : M, P, PT
paramsStable : P, PT

geometry : LHCb

@0
   name : Bs
@1
   name : Jpsi
@2
   name : phi
@3
   name : mup
   smear : LHCbGeneric
@4
   name : mum
   smear : LHCbGeneric
@5
```

```
    name : Kp
    smear : LHCbGeneric
    altMass : pi+
@6
    name : Km
    smear : LHCbGeneric
    altMass : pi-
```

where the @ notation is used to number the particles in the decay file, from left to right within each subdecay. Each particle can be given a unique **name** that is used to name the variables and histograms that are stored in the output data file. The effect of finite detector resolution is included through use of the **smear** keyword, typically only used for final state particles. By default, RapidSim includes momentum smearing parameterisations that can be applied to the generated four-vectors for pions, kaons, protons, muons (**LHCbGeneric**) or electrons (**LHCbElectron**). It is simple for the user to extend the available resolution parameterisations. The **altMass** keyword tells RapidSim to also compute the four-vector of the considered particle under a particle mass hypothesis that is different to the default mass. Appropriately named variables are added to the output file. The list of kinematic variables that RapidSim calculates for each of the decays and for each final state particle are defined at the head of the file using the **paramsDecaying** and **paramsStable** keywords.

5   Heavy quark production

5.1   FONLL

In producing a realistic simulation of decays at a hadronic collider, it is important to determine the kinematic distribution of the particles produced. RapidSim generates particles following a particle-gun-like approach — only the decaying particle is simulated, not the underlying event. This offers a significant time saving, but the kinematic distribution of the generated particles must be defined. RapidSim samples histograms generated from fixed-order next-to-leading-logarithm calculations [3] to determine the pseudorapidity, η, and transverse momentum, p_T, of the decaying particle. Example distributions are shown in Figure 1.

Histograms are included with the current version of RapidSim for the 4π production distributions of b- and c-hadrons in pp collisions at a range of centre-of-mass energies. The distribution used is configured at run time using the global option **energy** and the ID of the decaying particle. If necessary the **mother** option may be used to override the choice of histogram.

5.1.1   Custom production kinematics

Additional histograms may be saved to the **rootfiles/fonll/** directory. Each file must contain two **TH1** objects named **pT** and **eta** describing the differential production cross sections in transverse momentum and pseudorapidity, respectively. These may be obtained using the web interface provided at the URL in Ref [3]. Files using the naming scheme **LHC{flavour}{energy}.root** may be added without the need
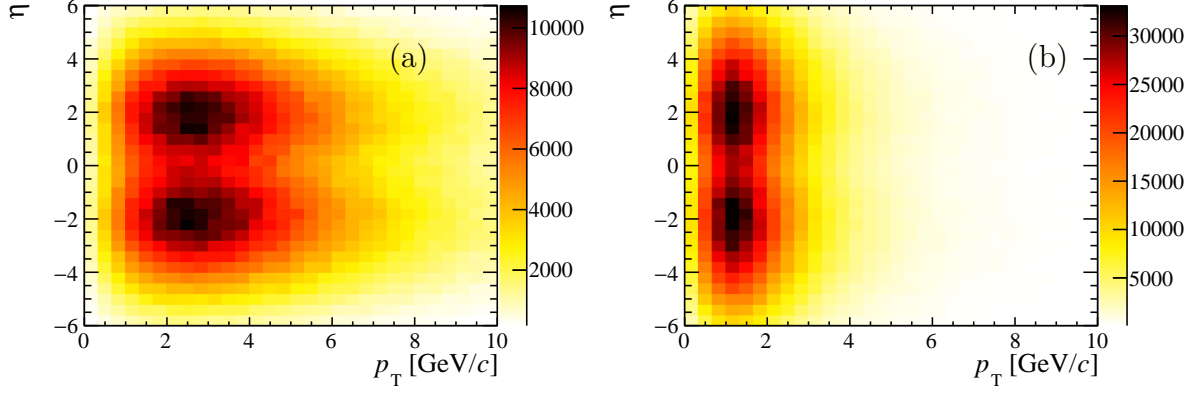
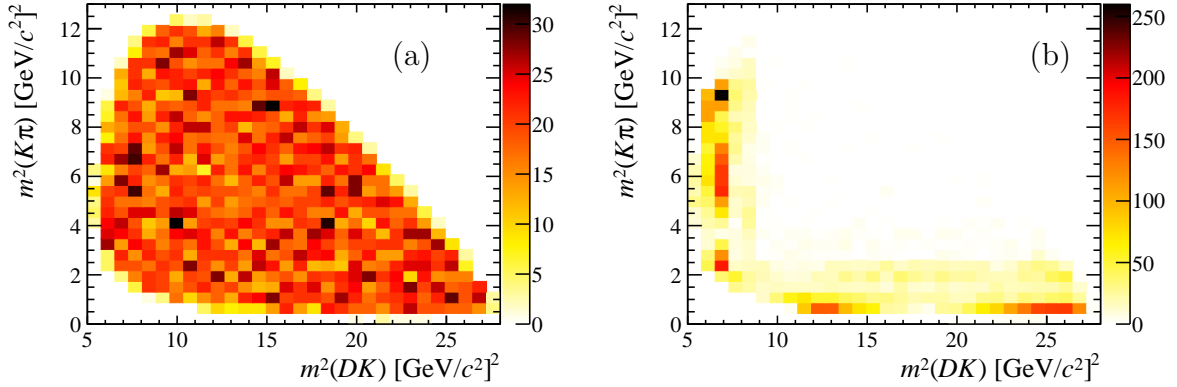Figure 1: Distribution in η and p_T of (a) B_s^0 mesons and (b) D^0 mesons produced in 7 TeV pp collisions.

Figure 2: Dalitz plots of $B_s^0 \to \bar{D}^0 K^- \pi^+$ (a) with a phase space distribution and (b) generated according to a 2D histogram.

to recompile the executable. Extensions to the naming scheme must be made in the `RapidConfig::loadParentKinematics` method.

5.2 Non-phase space distributions

By default, RapidSim generates all decays flat across the available phase space, however, in some cases it may be preferable to generate decays according to another distribution. RapidSim features the option to generate decays according to a one or two dimensional distribution in any defined parameters (see `param` option in Section 3). This is implemented via a Monte-Carlo accept/reject algorithm which is used to shape the initially generated phase-space distribution. Note that the requested number of events will be generated within the specified distribution, so inefficient accept/reject functions (such as a Dalitz plot with narrow resonances) will significantly increase the time required to generate each decay. An example is given in Figure 2. This option is configured at runtime using the `shape` global option, *e.g.* `shape : myFile.root myHisto M2_12 M2_23`.

6 Efficiency

RapidSim can account for two different types of efficiency: geometrical acceptance and selection requirements placed on kinematic quantities. These are detailed in Sections 6.1 and 6.2, respectively.

6.1 Geometrical acceptance

A requirement may be placed on the geometry of the decay. This may be configured via the configuration file at run time from a selection of defined options, however, new options must first be defined at compile time within the `RapidAcceptance` class. In the current version of the package, three LHCb-specific options are available in addition to the default:

Any No requirement is applied;

MotherIn The decaying particle is required to be within the angular acceptance of the LHCb detector;

AllIn All of the final-state particles are required to be within the angular acceptance of the LHCb detector;

AllDownstream All of the final-state particles are required to remain in the acceptance of the LHCb detector downstream of the dipole magnet.

The single acceptance requirement is configured using the global option `acceptance`, *e.g.* `acceptance : Any`. Figure 3 shows an example of the distribution of transverse momentum and pseudorapidity for B_s^0 mesons with each of the acceptance requirements applied.

6.2 Kinematic requirements

Selection requirements may be placed on any defined parameter (see `param` option in Section 3). Requirements may be a minimum (`min`); a maximum (`max`); a range (`range`); or an excluded range (`veto`) and are configured using the global option `cut`, *e.g.* `cut : pion_PT range 1 100`. An example is shown in Figure 4.

6.3 Missing particles

In certain decays some of the stable particles are not reconstructed (*e.g.* neutrinos in semi-leptonic decays or missing particles in partially reconstructed backgrounds). In such cases, it is of interest to reconstruct the mass or momentum of the parent particle excluding the momentum lost to the missing child particle. This may be reproduced in RapidSim using the `invisible` option. This option is turned on by default for neutrinos but may also be used for any other particle type. This option only affects reconstructed quantities — true quantities will account for the invisible particle. An example of this option is shown in Figure 5.
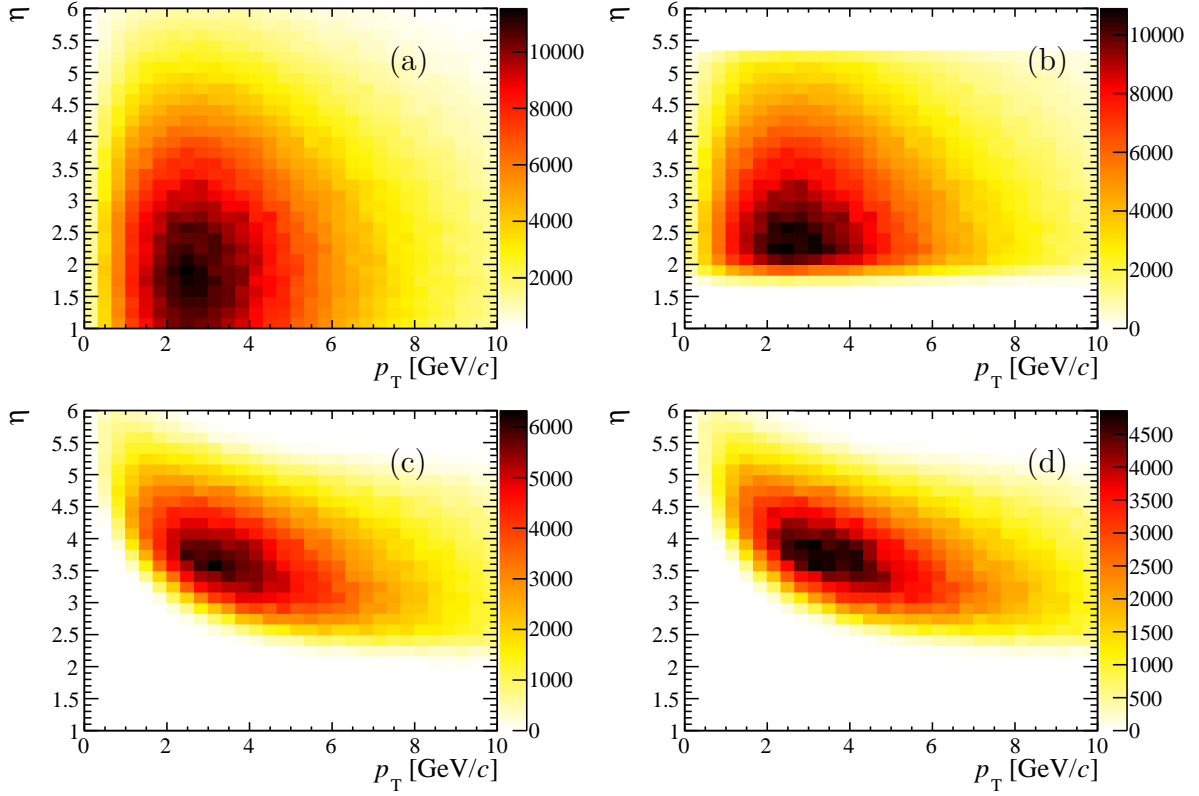
Figure 3: Distribution in η and p_{T} of B_s^0 mesons produced in 7 TeV pp collisions with (a) no acceptance requirement; (b) the B_s^0 meson required to be within the LHCb acceptance; (c) the decay products (from $B_s^0 \to J/\psi\,(\to \mu^+\mu^-)\phi\,(\to K^+K^-)$ decay) required to be within the LHCb acceptance; and (d) the decay products required to be within the LHCb acceptance downstream of the dipole magnet. nb by default, RapidSim only generates decays in the forward region $(1.0 < \eta < 6.0)$ when using the LHCb geometry.
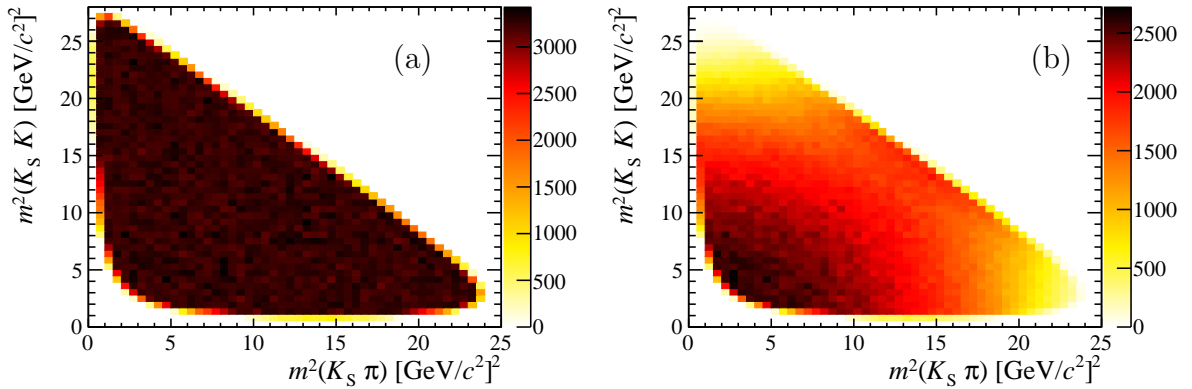

Figure 4: Example phase space Dalitz plot $(B_s^0 \to K_S^0 K^+\pi^-)$ with (a) no selection requirements and (b) p_{T} requirements on the kaon and pion to be larger than 1 GeV/c^2.
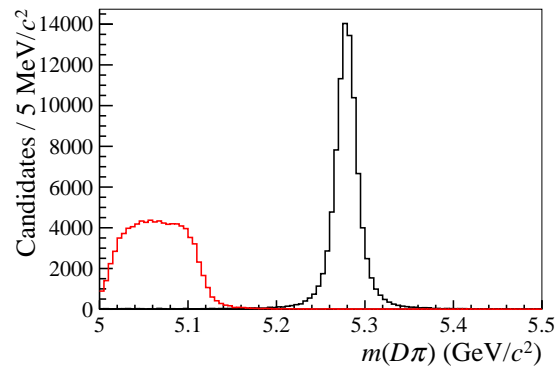
Figure 5: Distribution of $m(D\pi)$ invariant mass for (black) $D^0\pi^+$ decays where all particles are reconstructed and (red) $D^{*0}\pi^+$ decays where a neutral pion is missed.
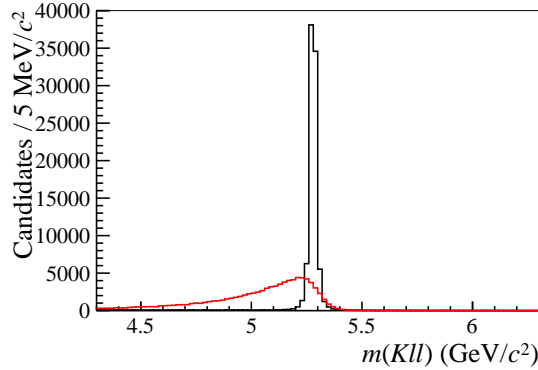
Figure 6: Simulated resolution effects on the distribution of $m(K^+l^+l^-)$ for B^+ mesons decaying to (black) $K^+\mu^+\mu^-$ and (red) $K^+e^+e^-$. The `LHCbGeneric` smearing option has been used for the kaon and muons, while the `LHCbElectron` option (which accounts for Bremsstrahlung) has been used for the electron and positron.

7 Momentum smearing

RapidSim simulates the effect of a finite momentum resolution by smearing the momentum of each stable particle according to a defined resolution function. Smearing options are defined in the `config/smear/` directory (as described in Section 7.1) and configured for each particle using the `smear` keyword. Resolution functions may be defined either by a Gaussian distribution with a p-dependent (or p_{T}- and η-dependent) width, or by a series of histograms that describe the resolution in different p ranges. The former approach allows the width of the resolution function to vary continuously and is the best option in most cases. The predefined `LHCbGeneric` smearing option uses this approach to model the resolution effects on charged hadrons and muons in the LHCb experiment, based on the calibration documented in Refs. [6,7]. The histogram-based approach allows for asymmetric effects such as Bremsstrahlung to be modelled and is used in the predefined `LHCbElectron` option, which is based on a modified version of the model given in the supplementary material of Ref. [8]. Examples of these two smearing options are shown in Figure 6. The `AtlasHadron` and `AtlasMuon` options use the momentum resolution calibration from Ref. [9] to model the resolution effects as a function of p_{T} and η in the ATLAS experiment for hadrons and muons. It is assumed that the resolution for hadrons is uniform as a function of p_{T}, which is reasonable for tracks with $p_{\mathrm{T}} > 1\,\mathrm{GeV}/c$.

Figure 7 shows examples of the distributions of $J/\psi K^+$ invariant mass in selected $B^+ \to J/\psi K^+$ decays from the LHCb and ATLAS experiments and the corresponding signal-only distributions generated using RapidSim with the relevant momentum smearing options enabled. The RapidSim simulation manages to reproduce the mass resolution observed in data.

7.1 Configuration

Each smearing option is defined by a single ASCII configuration file and a single ROOT file containing either a `TGraph` object (for Gaussian resolution options with a p-dependent width), a `TH2` object (for Gaussian resolutions with p_{T} and η dependence), or one or more
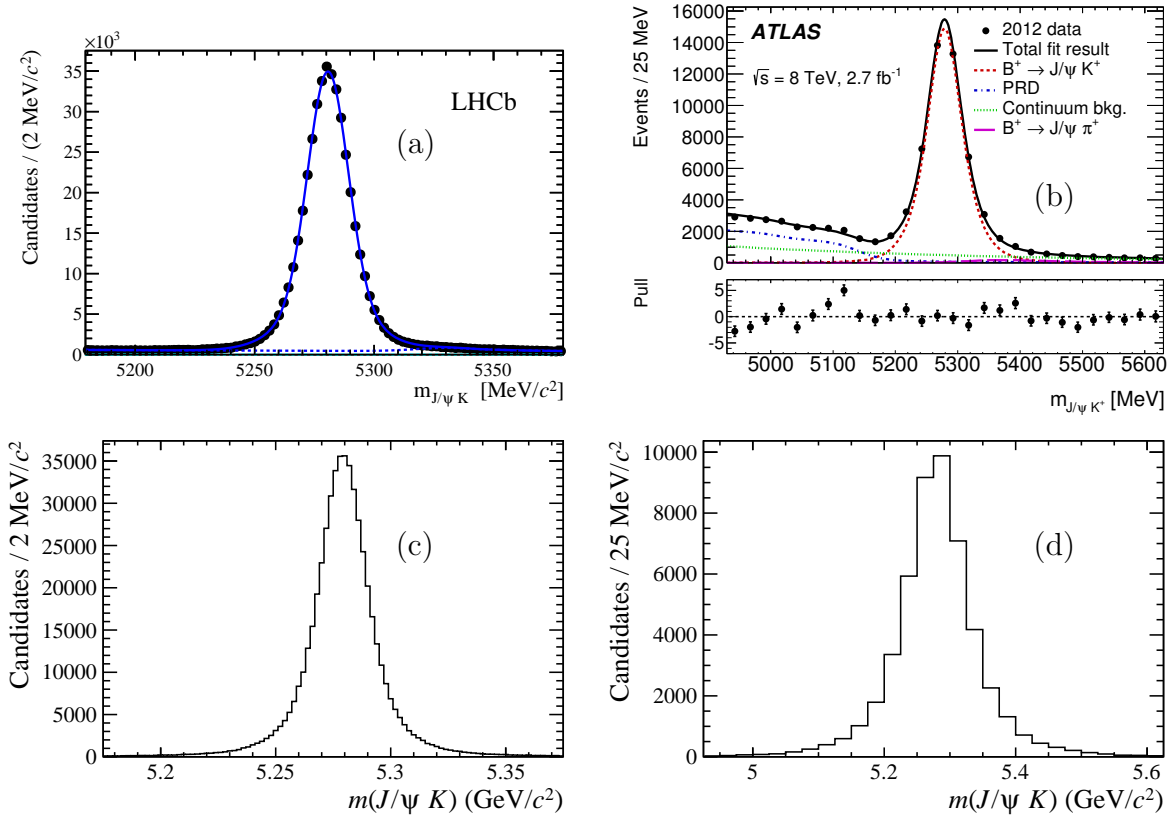
Figure 7: Distributions of the invariant mass of $B^+ \to J/\psi\, K^+$ decays in the (a) LHCb [10] and (b) ATLAS [11] experiments and those generated by RapidSim for (c) LHCb conditions and (d) ATLAS conditions. Note the different scales on the abscissas.

TH1 objects (for histogram-based options). The configuration file is formatted as follows:

- The first line gives the path to the associated ROOT file.

- The second line is GAUSS for p-dependent Gaussian smearing options, GAUSSPTETA for p_{T}- and η-dependent Gaussian smearing options, and HISTS for histogram smearing options.

- For Gaussian smearing options, the third line gives the name of the TGraph (TH2) object that gives the resolution width as a function of p (p_{T} and η).

- For histogram smearing options, the third and subsequent lines give the lower edge of a p bin and the name of the TH1 object describing the resolution function in that bin. An example file is given below.

```
electronHists.root
HISTS
0       P0_hist
10000   P1_hist
15000   P2_hist
20000   P3_hist
```
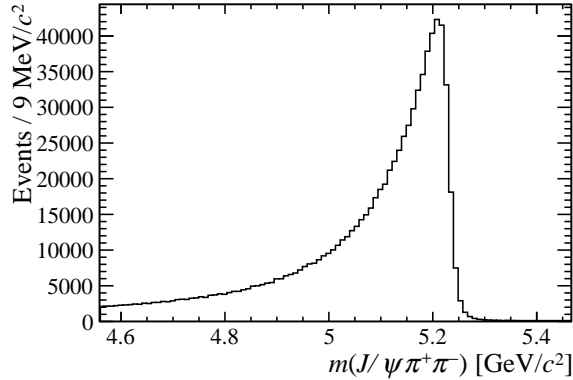
Figure 8: Distribution of $J/\psi\pi^+\pi^-$ invariant mass for $B_s^0 \to J/\psi\phi$ decays where both kaons have been mis-identified as pions.

```
30000    P4_hist
50000    P5_hist
```

8   Particle mis-identification

RapidSim can also calculate quantities using an alternative mass hypothesis for one or two particles. This is particularly useful when investigating backgrounds where a particle has been mis-identified. Multiple alternative mass hypotheses may be defined for each particle using the particle's `altMass` option (*e.g.* `altMass :   K+ mu+` will add both kaon and muon masses as alternative hypotheses). All parameters will be calculated for all combinations of hypotheses with two or fewer mis-identified particles. For instance, $D^0 \to K^-\pi^+$ with $\pi \to \mu$, $\pi \to K$ and $K \to \pi$ mis-identifications considered will result in a total of five alternative mass hypotheses ($K^-\mu^+$, K^+K^-, $\pi^-\pi^+$, $\pi^-\mu^+$ and π^-K^+). Figure 8 shows an example mass distribution calculated with mis-identifications of two final state particles.

9   Summary

A common task in the analysis of heavy-flavour hadron decays at particle physics experiments is to understand the kinematic properties of the signal and background processes, in particular when determining selection requirements or when describing the invariant mass spectrum of the final state particles. RapidSim is a new lightweight application that allows the analyst to quickly generate specific heavy-flavour hadron decays with realistic production kinematic distributions, efficiencies and momentum resolutions. The specific decay properties and options are controlled via simple user-defined configuration files. The production environment, momentum resolutions and desired efficiency are defined via externally provided parameterisations. The simple framework allows the user to easily extend the simulation should more detail be required, such as the addition of alternative detector geometries beyond the defaults provided. The problem of understanding the shape of hadron decays where one or more of the final state particles are mis-identified is

handled in a simple way via a configuration file. Altogether, RapidSim packages many aspects of typical particle physics analyses into a simple application that gives users the ability to rapidly generate large samples of decays that can be used to aid their understanding without the need to generate fully simulated decays and the corresponding use of computing and storage resources that it entails. It is already being utilised in ongoing analyses within the LHCb collaboration.

Acknowledgements

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