Systematics with pyhf

Karlsruhe Institute of Technology

Institute of Experimental Particle Physics

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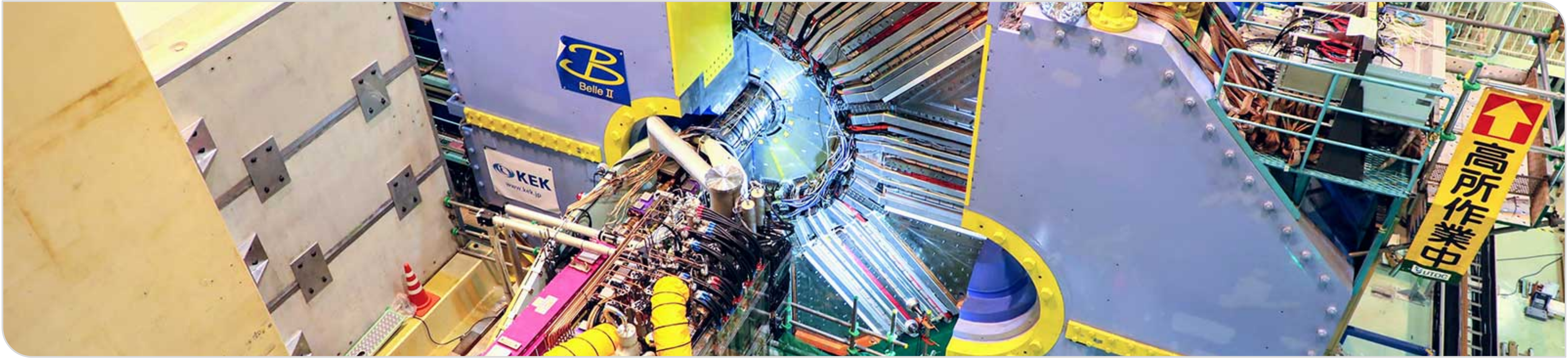
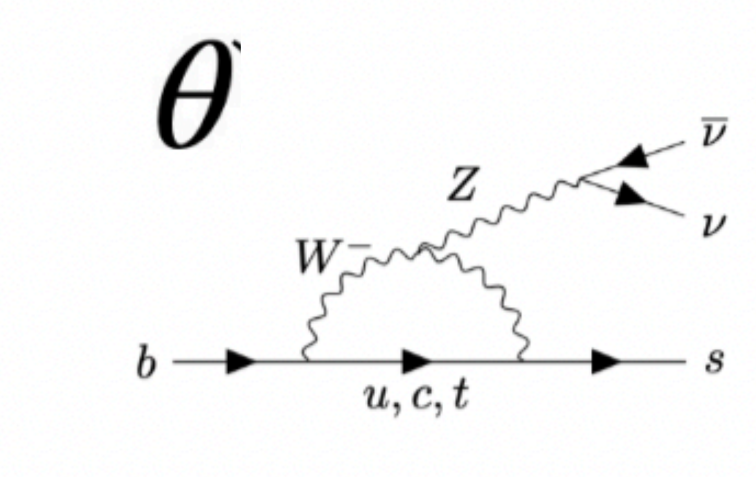
Slavomira Stefkova (KIT), Lorenz Gärtner (LMU)

slavomira.stefkova@kit.edu

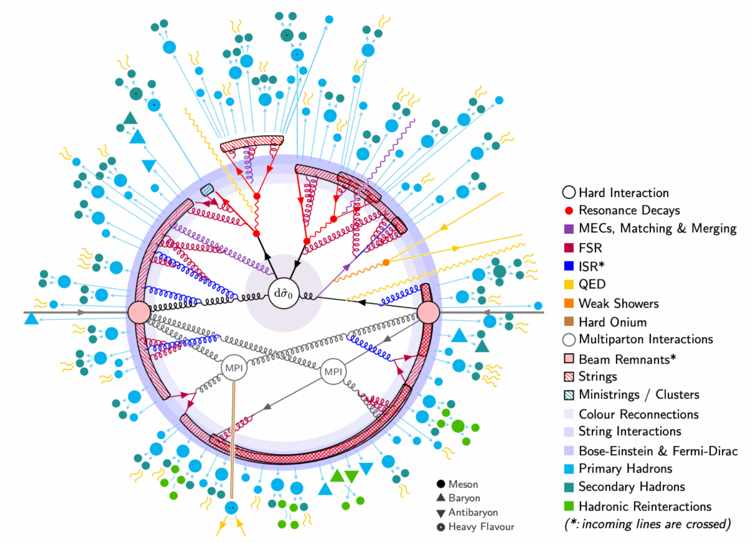


What we want to do?

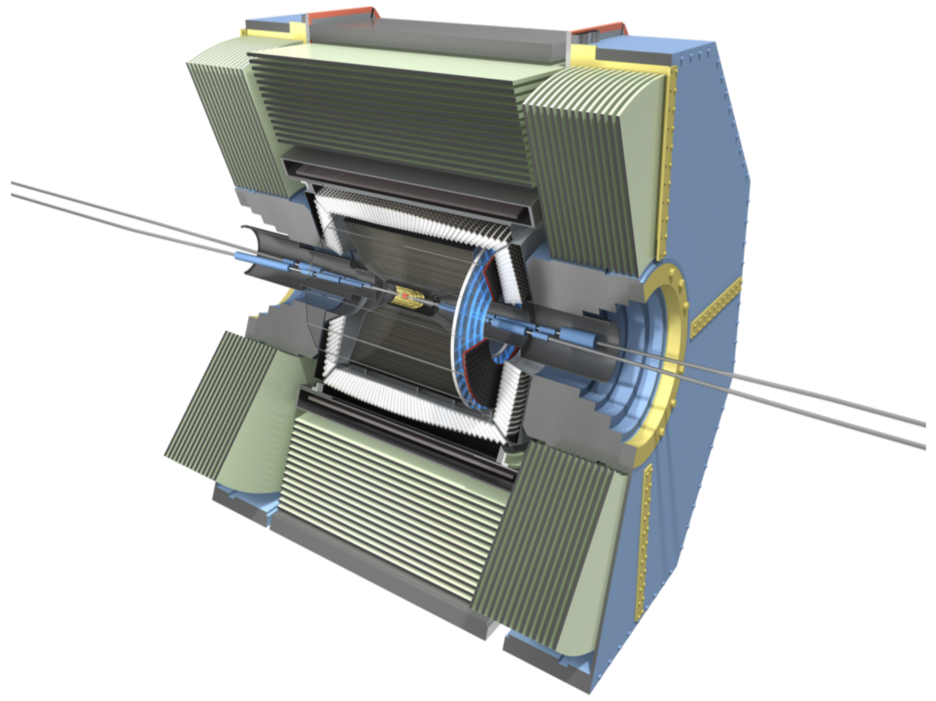
Simulation of signal and background physics processes



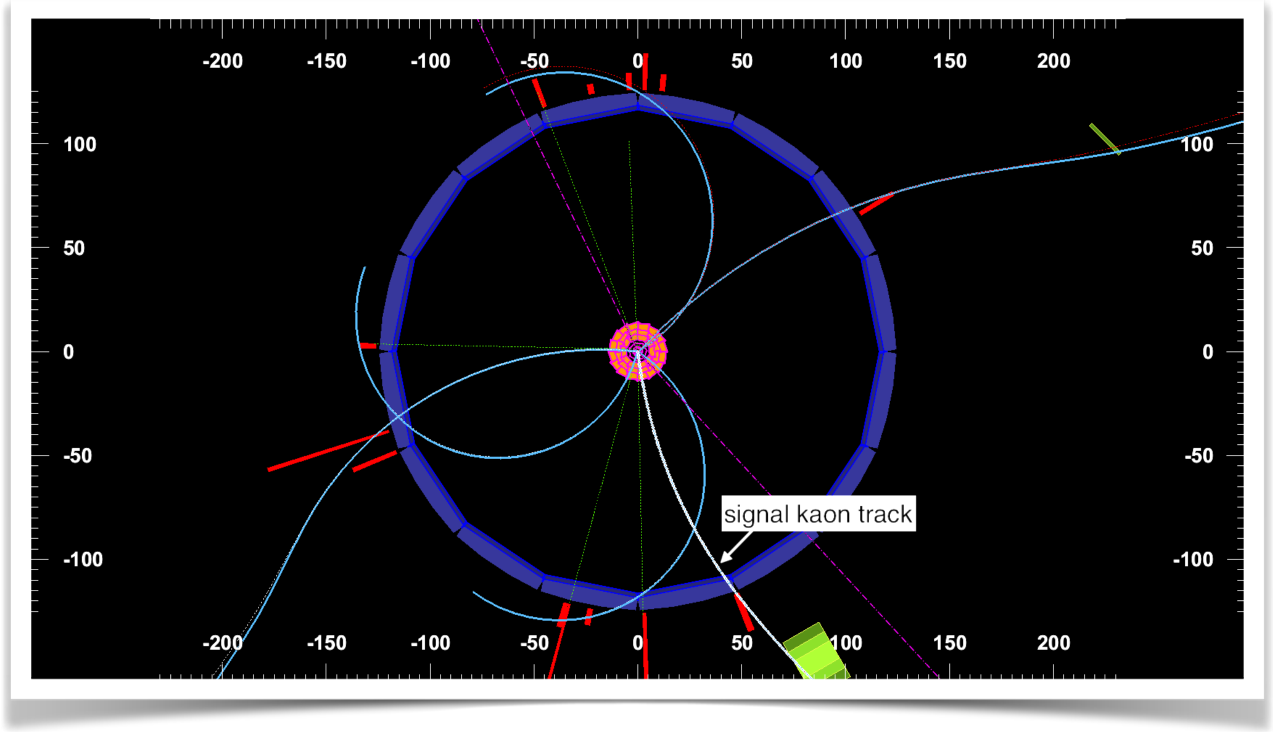
Simulation of stochastic evolution



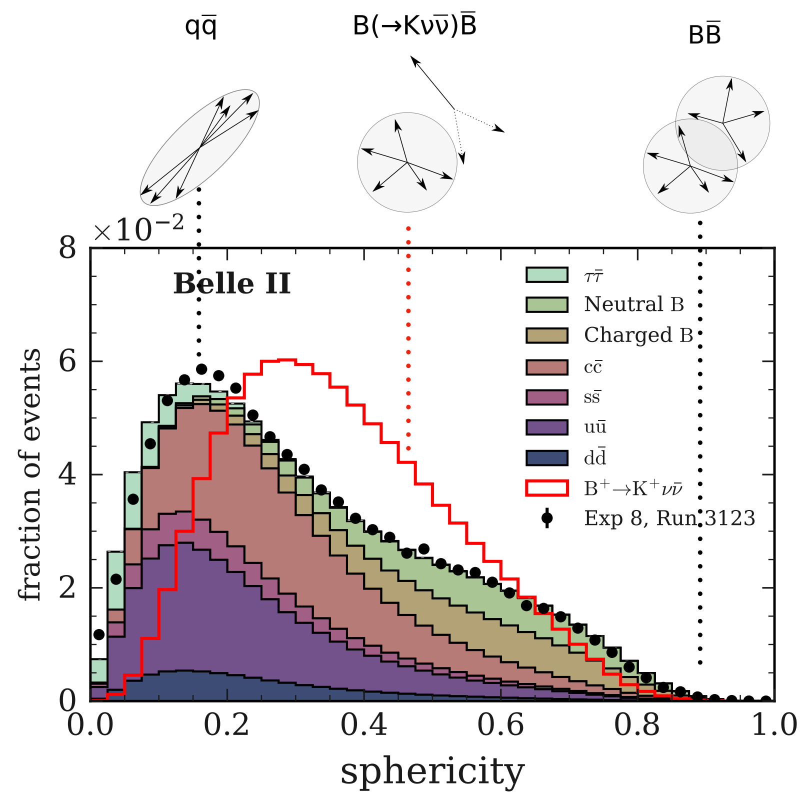
Simulation of Belle II detector and its readout



Belle II reconstruction

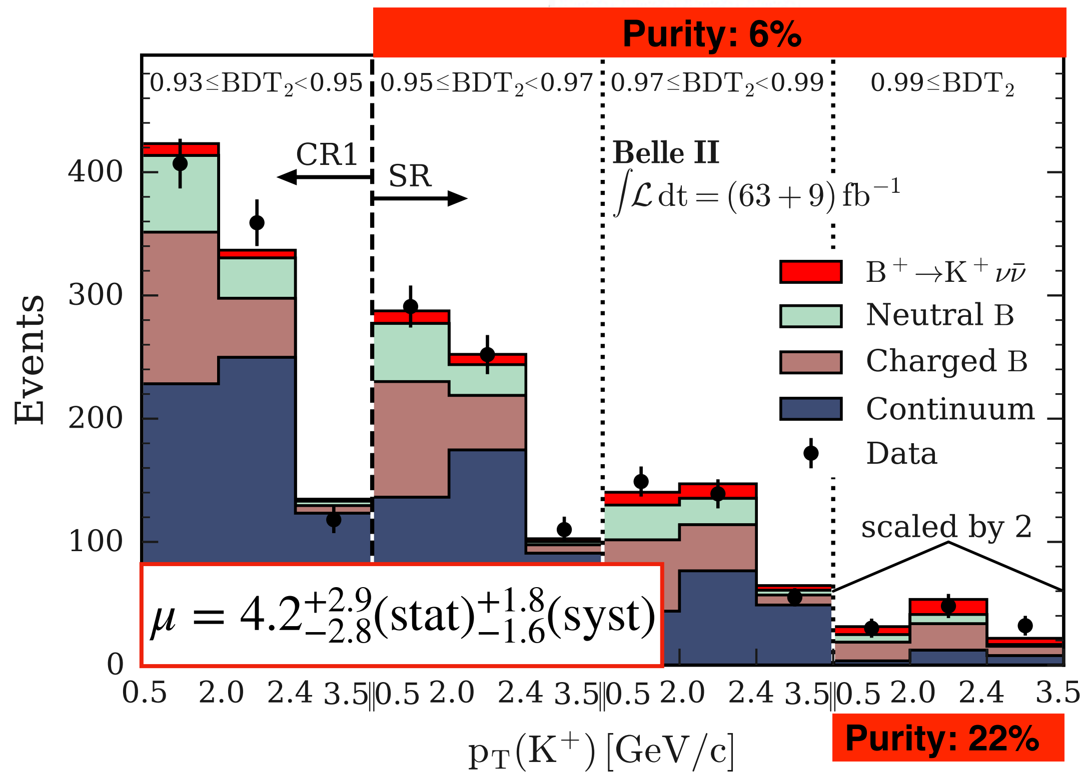


Analysis event selection



Fitting distributions

data

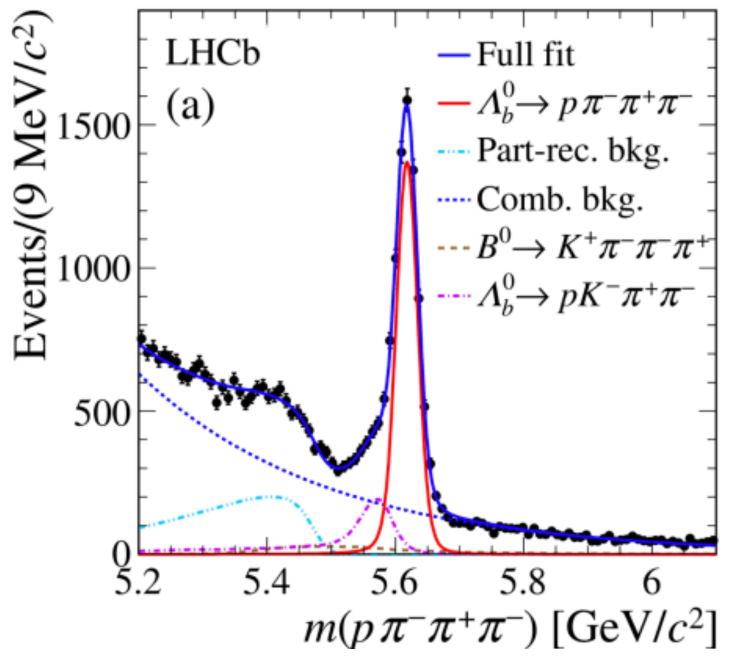


$$p(\text{data} \mid \theta)$$

Model-building

Model Description →

Unbinned

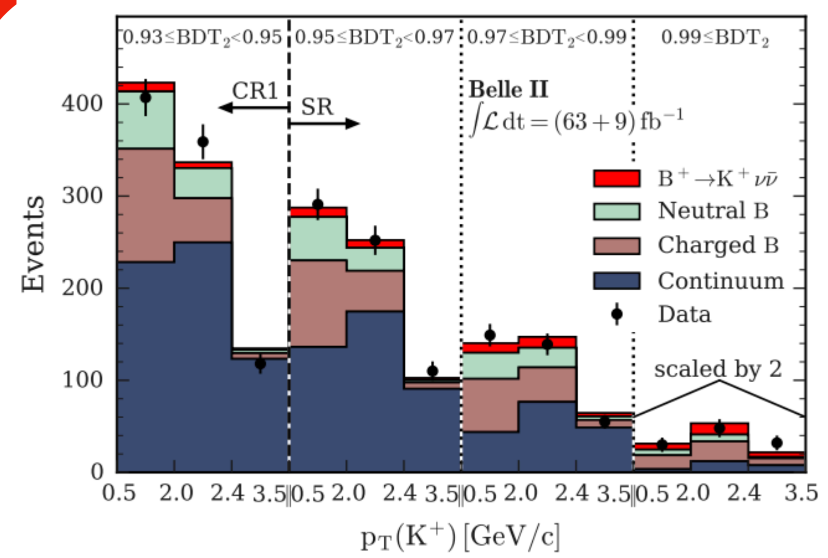


Per-event model

$$p(\{x_i\}\,|\,\theta) = \text{Pois}(N\,|\,\theta)\prod_{i=0}^{N} p(x_i\,|\,\theta)$$

Parametrised functions: (Crystal Balls, exponential, Gauss, …) Density Estimates (KDE)

Binned



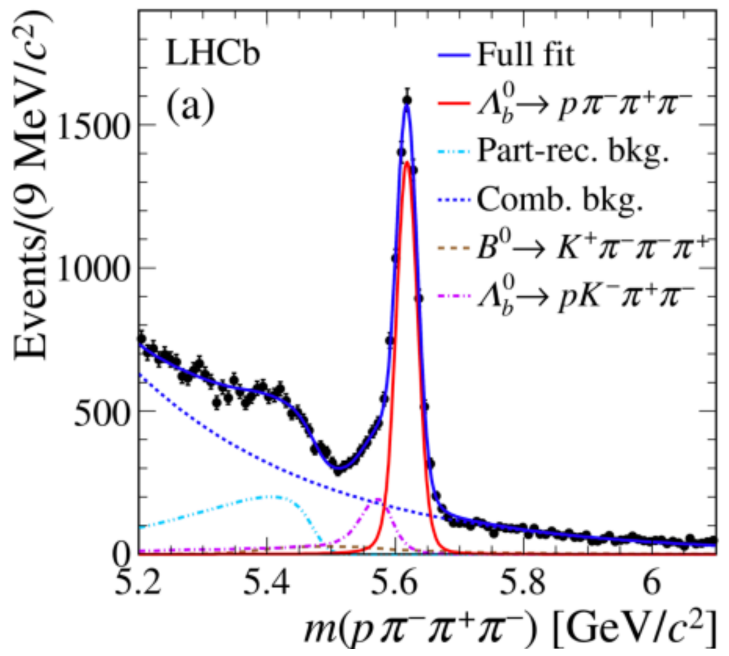
Step-wise per-event model

$$p(\{n_b\}\,|\,\theta) = \prod_b \text{Pois}(n_b\,|\,\lambda(\theta)p(b\,|\,\theta)) = \prod_b \text{Pois}(n_b\,|\,\lambda_b(\theta))$$

Parametrised histograms

Model-building and fitting

Unbinned



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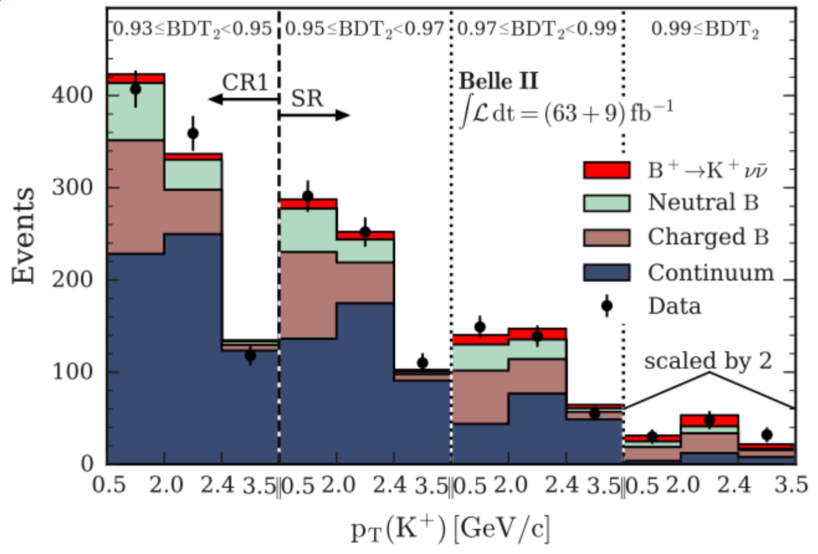

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Model Description

Parametrised functions: (Crystal Balls, exponential, Gauss, …) Density Estimates (KDE)

Parametrised histograms

Fitting

Maximum Likelihood Fit

$$L(\mu, \vec{\theta})$$

Limit Setting

- Frequentist
  - Asymptotic
  - Toy-based
- Bayesian

$$\lambda(\mu) = \frac{\mathcal{L}(\mu, \hat{\hat{\theta}})}{\mathcal{L}(\hat{\mu}, \hat{\theta})}$$

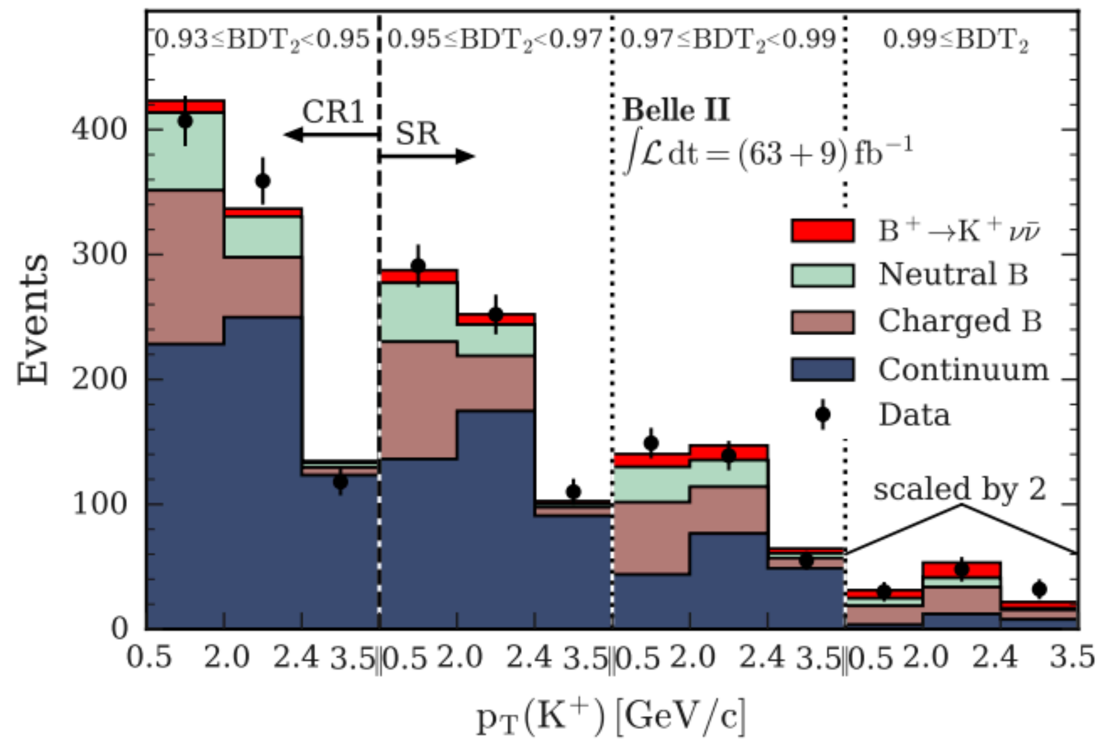
Observation

- Significance

Fitting variables and POI

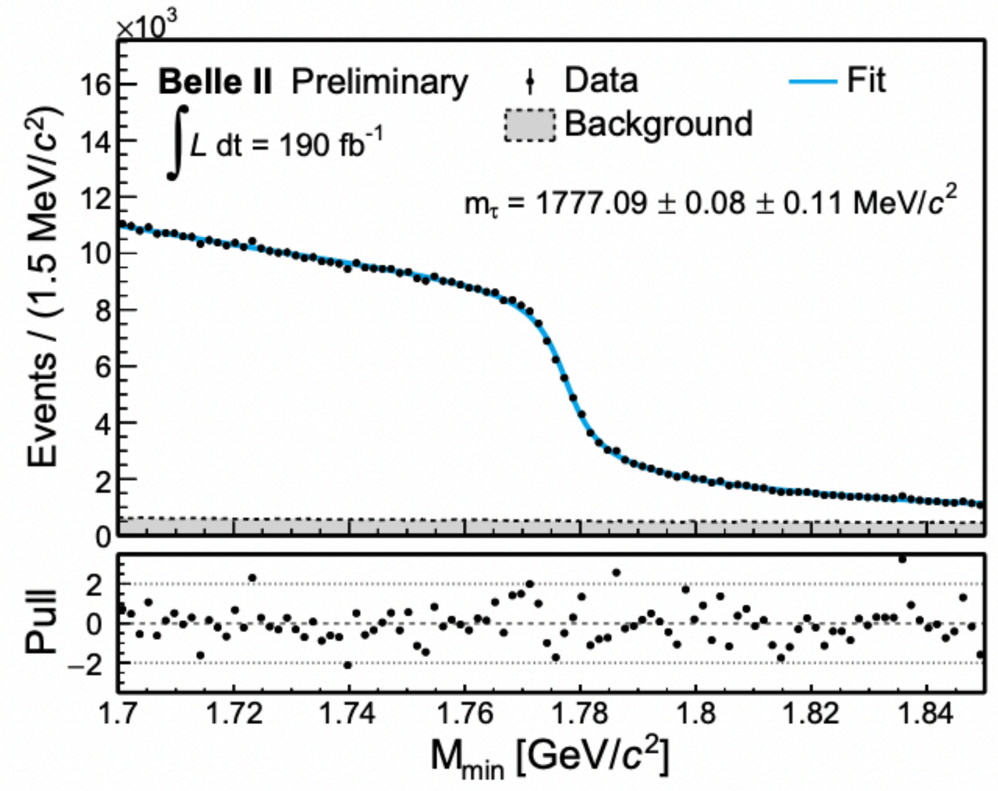
In general we want to perform fit to **(kinematic) variables (observables)** where there is a **separation between signal and background** after all the selection:

1. ΔE, M_{bc} , Δt for fully reconstructed decays
2. $E_{missing}$ for non-fully reconstructed decays
3. MVA classifiers



With fit we want to measure our **parameter of interests (POI):**

- Branching fractions
- *S, A,* lifetimes
- masses of elementary particles (e.g τ)



Fitting (libraries)

We can code everything from scratch (your own) or there are libraries which have developed efficient ways that include all the functionalities of fitting:

What HEP fitting libraries do we have?

1. Unbinned: your own, zfit, *RooFit*
2. Binned: your own, zfit, *RooFit*, pyhf

https://indico.belle2.org/event/7653/timetable/#20221007

In addition, in HEP we usually perform statistical interpretation of the results:

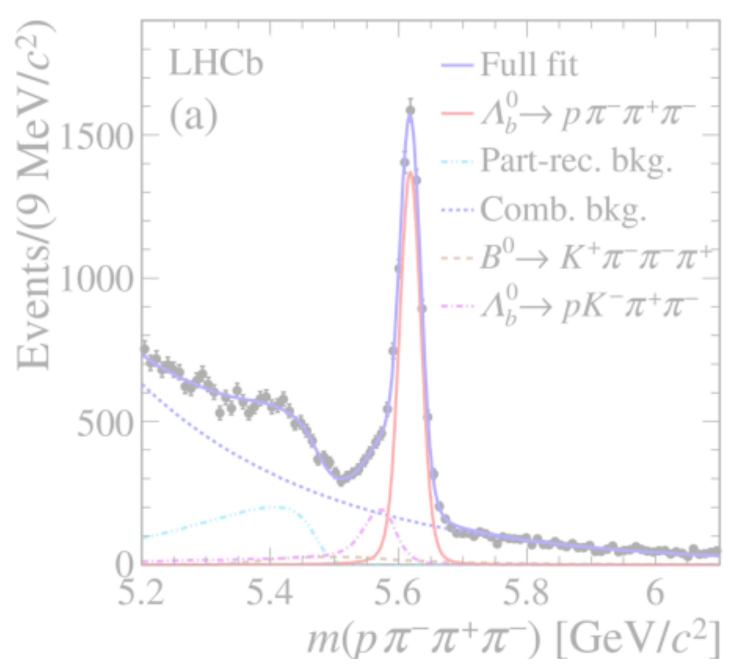
- *RooStats*, zfit, pyhf, your own

When do we use binned fits?

- Either statistics is too little or too large
- When there is no parametric description of your distribution
- For 1D distr. binned fits are faster and more numerically stable, for 2D the opposite is true

Model-building (Binned)

Unbinned



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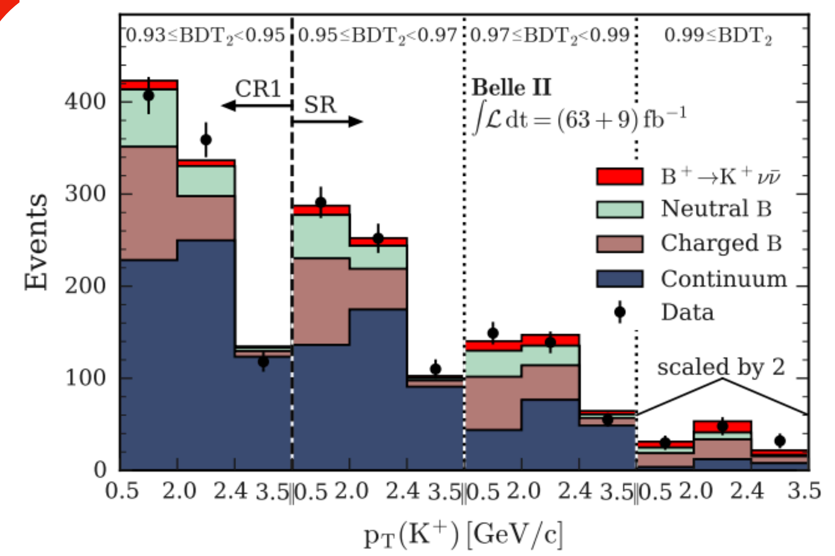

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Model Description

Parametrised functions: (Crystal Balls, exponential, Gauss, …) Density Estimates (KDE)

Parametrised histograms

Pyhf

pyhf

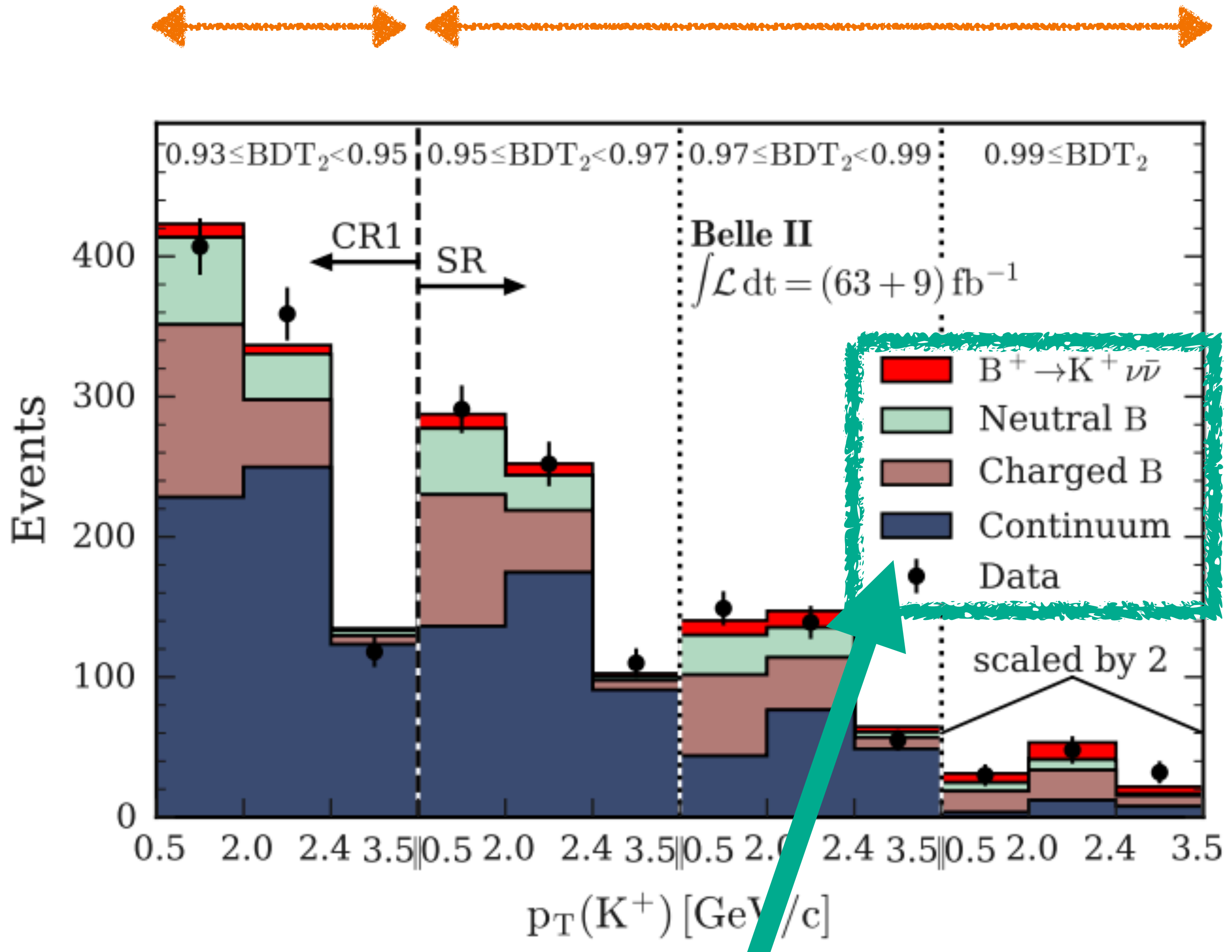
- Pure python library used for fitting and statistical interpretation of binned templates
- Based on HistFactory formalism (traditionally used with *RooFit*, and *RooStats*)
- Main model configuration in simple-to-read and industry-state JSON format

pyhf and Belle II:

- We already had 1st Belle II pyhf workshop on 03/03/2023, see more details in https://indico.belle2.org/event/8470/
- **Today we want to give tutorial that covers**
    - **Systematics and pyhf**
    - **Systematics in Belle II**
    - **How to implements systematics in Belle II in practice**

HistFactory Formalism

Channels = disjoint measurement regions eg. signal region, control region



Samples = physics processes

$$f(\boldsymbol{x}|\boldsymbol{\phi}) = f(\boldsymbol{x}|\overbrace{\boldsymbol{\eta}}^{\text{free}}, \underbrace{\boldsymbol{\chi}}_{\text{constrained}}) = f(\boldsymbol{x}|\overbrace{\boldsymbol{\psi}}^{\text{parameters of interest}}, \underbrace{\boldsymbol{\theta}}_{\text{nuisance parameters}})$$

$$f(\boldsymbol{n}, \boldsymbol{a}\,|\,\boldsymbol{\eta}, \boldsymbol{\chi}) = \underbrace{\prod_{c \in \text{channels}} \prod_{b \in \text{bins}_c} \text{Pois}\left(n_{cb}\,|\,\nu_{cb}(\boldsymbol{\eta}, \boldsymbol{\chi})\right)}_{\text{Simultaneous measurement of multiple channels}} \underbrace{\prod_{\chi \in \boldsymbol{\chi}} c_{\chi}(a_{\chi}|\,\chi)}_{\text{constraint terms for "auxiliary measurements"}}$$

$$\nu_{cb}(\boldsymbol{\phi}) = \sum_{s \in \text{samples}} \nu_{scb}(\boldsymbol{\eta}, \boldsymbol{\chi}) = \sum_{s \in \text{samples}} \underbrace{\left(\prod_{\kappa \in \boldsymbol{\kappa}} \kappa_{scb}(\boldsymbol{\eta}, \boldsymbol{\chi})\right)}_{\text{multiplicative modifiers}} \left(\nu_{scb}^{0}(\boldsymbol{\eta}, \boldsymbol{\chi}) + \underbrace{\sum_{\Delta \in \boldsymbol{\Delta}} \Delta_{scb}(\boldsymbol{\eta}, \boldsymbol{\chi})}_{\text{additive modifiers}}\right)$$

Main ingredients:

- Main Poissonian pdf
- Constraint pdf (+ data) for auxiliary measurements
- n_{cb} observed events, ν_{cb} event rates, ν_{sbc}^{0} nominal rates, a_{χ} auxiliary data, $\vec{\eta}$ unconstrained pars, $\vec{\chi}$ unconstrained pars

HistFactory: systematics

Description	Modification	Constraint term c_χ	Input	Type	"Data field"	Factor
Uncorrelated shape	$\kappa_{scb}(\gamma_b) = \gamma_b$	$\prod_b \text{Pois}\left(r_b = \sigma_b^{-2} \middle\| \rho_b = \sigma_b^{-2}\gamma_b\right)$	σ_b	shapesys	Per-bin	Bin-wise
Correlated shape	$\Delta_{scb}(\alpha) = f_p\left(\alpha \middle\| \Delta_{scb,\alpha=-1}, \Delta_{scb,\alpha=1}\right)$	$\text{Gaus}\left(a = 0 \middle\| \alpha, \sigma = 1\right)$	$\Delta_{scb,\alpha=\pm1}$	histosys	Per-bin	Global
Normalisation uncertainty	$\kappa_{scb}(\alpha) = g_p\left(\alpha \middle\| \kappa_{scb,\alpha=-1}, \kappa_{scb,\alpha=1}\right)$	$\text{Gaus}\left(a = 0 \middle\| \alpha, \sigma = 1\right)$	$\kappa_{scb,\alpha=\pm1}$	normsys	Per-sample	Global
MC stat uncertainty	$\kappa_{scb}(\gamma_b) = \gamma_b$	$\prod_b \text{Gaus}\left(a_{\gamma_b} = 1 \middle\| \gamma_b, \delta_b\right)$	$\delta_b^2 = \sum_s \delta_{sb}^2$	staterror	Per-bin	Bin-wise
Luminosity	$\kappa_{scb}(\lambda) = \lambda$	$\text{Gaus}\left(l = \lambda_0 \middle\| \lambda, \sigma_\lambda\right)$	$\lambda_0, \sigma_\lambda$	lumi	–	Global
Normalisation	$\kappa_{scb}(\mu_b) = \mu_b$	–	–	normfactor	–	Global
Data-driven shape	$\kappa_{scb}(\gamma_b) = \gamma_b$	–	–	shapefactor	–	Bin-wise

Seven different systematic types:

- Correlated shape (bin-by-bin)
- Uncorrelated shape (bin-by-bin)
- MC Stat. uncertainty: uncertainty due to the finite sample size of the datasets
- Normalisation-related systematics: Normalisation, Luminosity, Normalisation uncertainty
- Systematics can affect both shape and normalisation: share the name to correlate them
- Systematics can affect different samples: share the name of the modifier to correlate them

HistFactory: systematics

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JSON Format Example: Input File

Four main parts

- Channels: description of the samples + their possible parametrised modifiers
- Observations: observed data
- Measurements: define parameter of interest (POI) and other measurements
- Version: specification of JSON version

Simple syntax which encodes the model in JSON format!

```
{
    "channels": [ # List of regions
        { "name": "singlechannel",
          "samples": [ # List of samples in region
            { "name": "signal",
              "data": [20.0, 10.0],
              # List of rate factors and/or systematic uncertainties
              "modifiers": [ { "name": "mu", "type": "normfactor", "data": null} ]
            },
            { "name": "background",
              "data": [50.0, 60.0],
              "modifiers": [ {"name": "uncorr_bkguncrt", "type": "shapesys", "data": [5.0, 12.0]} ]
            }
          ]
        }
    ],
    "observations": [ # Observed data
        { "name": "singlechannel", "data": [55.0, 62.0] }
    ],
    "measurements": [ # Parameter of interest
        { "name": "Measurement", "config": {"poi": "mu", "parameters": []} }
    ],
    "version": "1.0.0" # Version of spec standard
}
```

- **Two samples: signal [20, 10] + background [50, 60]**
- **Observed data [55, 62]**

Very simple example

$$f(\boldsymbol{n}, \boldsymbol{a} \mid \boldsymbol{\eta}, \boldsymbol{\chi}) = \underbrace{\prod_{c \in \text{channels}} \prod_{b \in \text{bins}_c} \text{Pois}\left(n_{cb} \mid \nu_{cb}(\boldsymbol{\eta}, \boldsymbol{\chi})\right)}_{\text{Simultaneous measurement of multiple channels}} \underbrace{\prod_{\chi \in \boldsymbol{\chi}} c_\chi(a_\chi \mid \chi)}_{\text{constraint terms for "auxiliary measurements"}}$$

Simple two-bin two-sample scenario

- Two samples: signal [20, 10] + background [50, 60]
- Signal with no uncertainty: unconstrained μ (POI)
- Background with two uncorrelated shape systematics: γ_1 and γ_2 (10% and 20%)
- Required input is σ_b = relative uncertainty of this modifier → data=[5,12]

$$\begin{aligned} p_{\text{main}} \cdot p_{\text{aux}} &= \text{Pois}(n|\lambda) \cdot p_{\text{aux}} \\ &= \text{Pois}(n|\mu s + \gamma b) \cdot p_{\text{aux}} \\ &= \boxed{\text{Pois}(n|\mu s + \gamma b)} \cdot \boxed{\text{Pois}(n_{\text{aux}} = (b/\delta b)^2 | \mu = (b/\delta b)^2 \gamma)} \end{aligned}$$

HistFactory: systematics

- Seven different systematic types

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Few words about systematics in general

The good, bad and ugly

The Good: calibrations, basically statistical

The Bad: using other peoples results, poorly modelled data or analysis technique, model assumptions,….

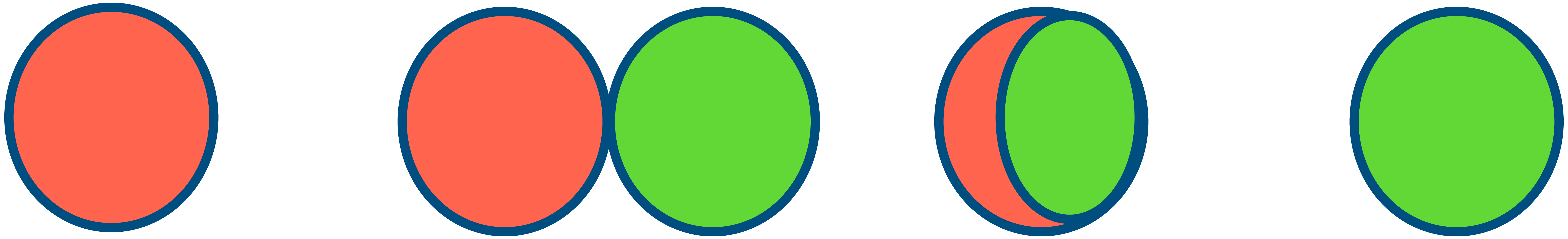
The Ugly: different theoretical estimates, …

Credits to PHYSTAT forum

→ Systematic uncertainties can affect shape, normalisation or both

What samples do we use for systematics?

1. Alternative models (simulation)
2. Calibration samples (mixture of simulation and data)
3. Signal/background embedding samples (mixture of simulation and data)
4. *(Orthogonal) data samples (data)*



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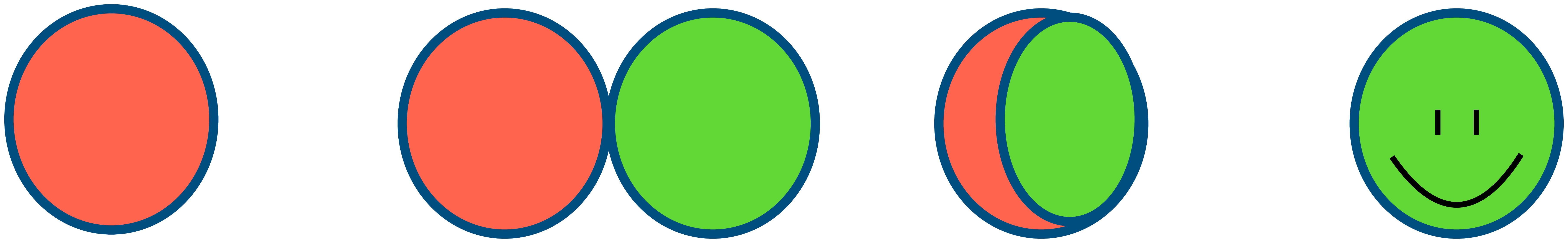


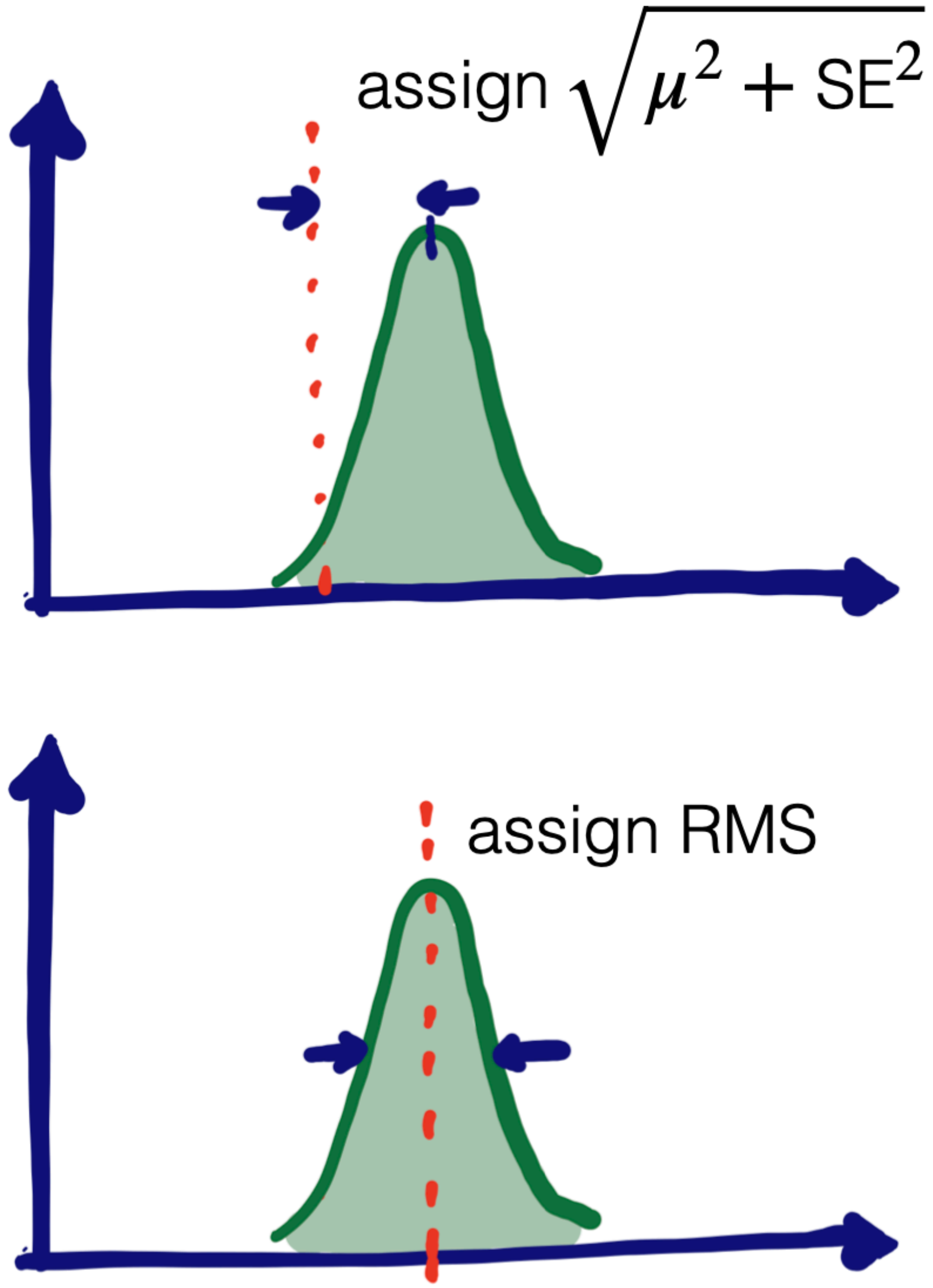
The best Monte Carlo is the data!

How do we get systematic variations?

What methods do we use? [T.Blake (Phystat 2021)]:

1. Generate a large number of pseudo-experiments from a varied model and determine observables using the nominal model…(bootstrap / toy method)
2. Repeat the determination of the observables in data / simulation using a different set of assumptions… (alternative method)

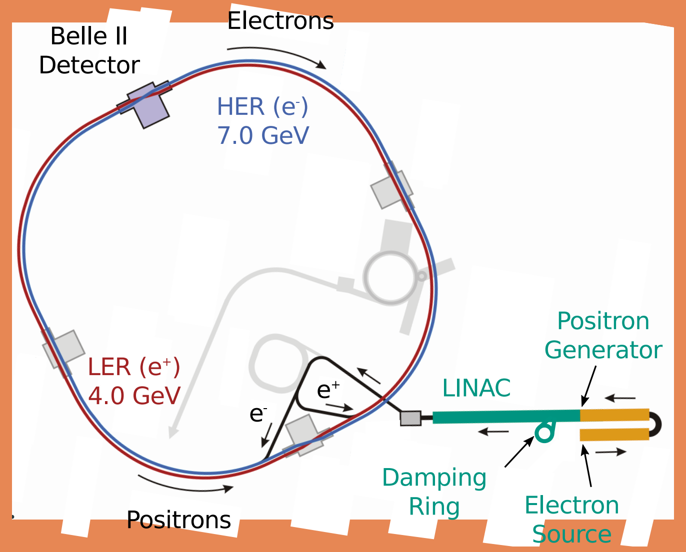
→ **Systematic uncertainties can affect shape, normalisation or both**



Systematic uncertainties @ Belle II

Types of systematic uncertainties

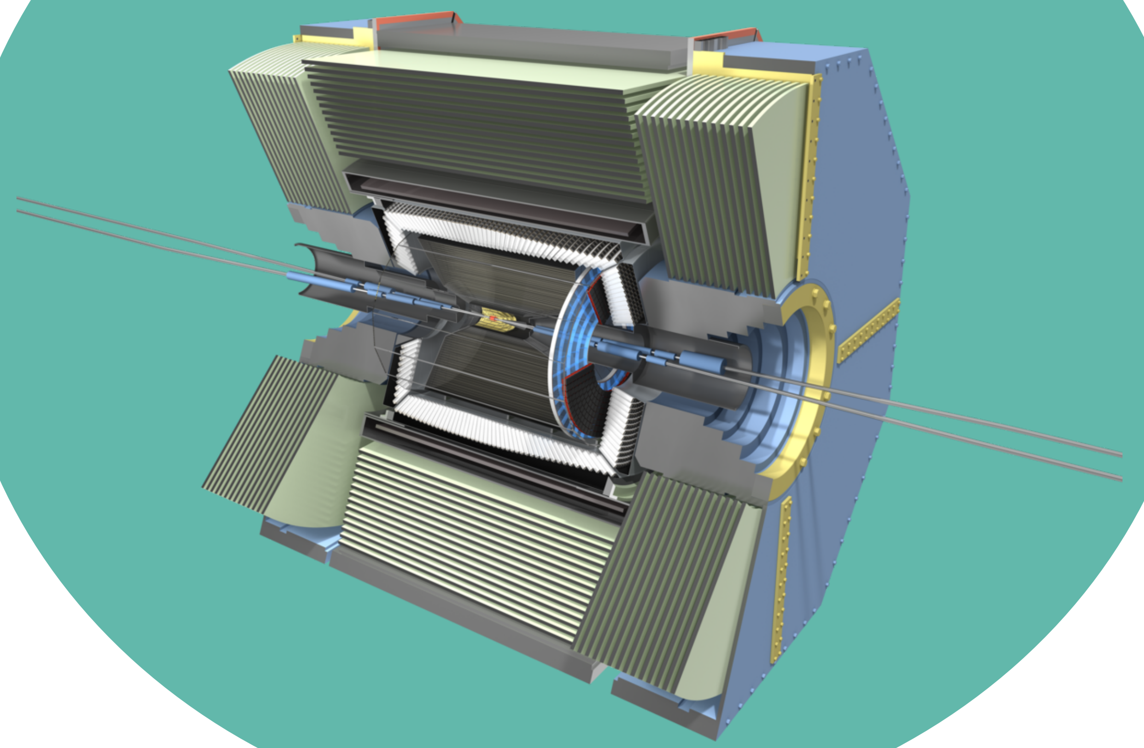
Accelerator



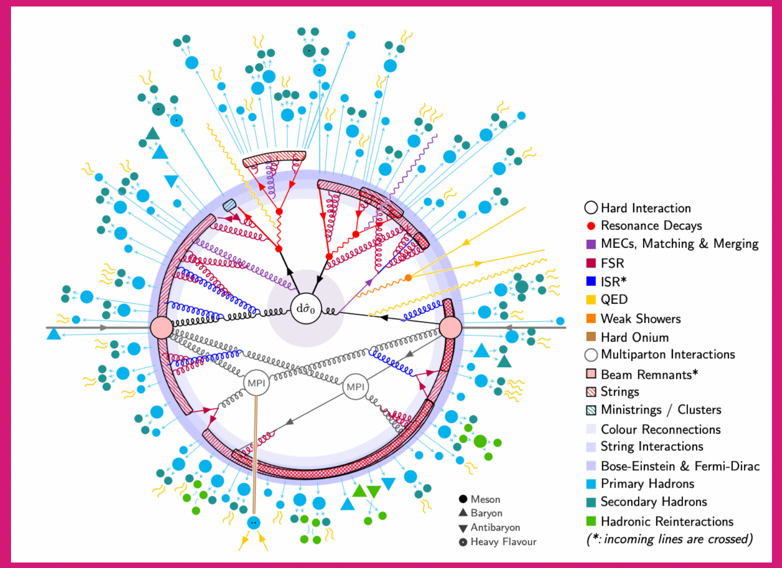
External Measurement

BESIII

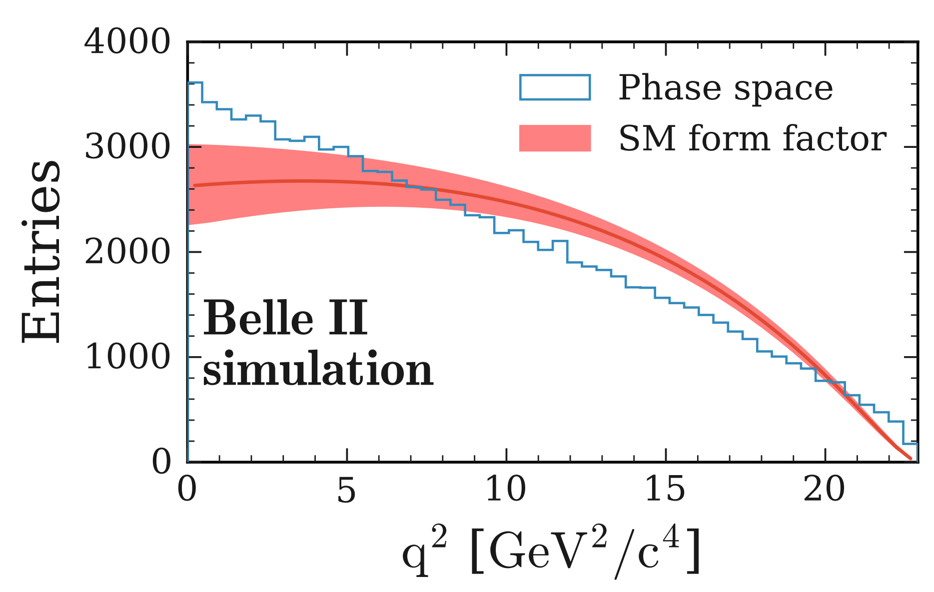
Detector



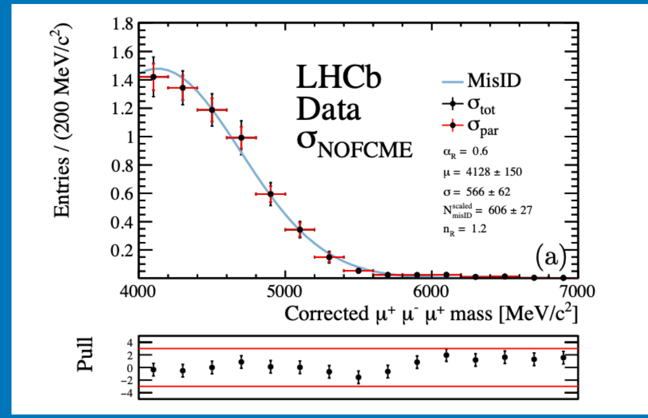
Simulation



Theory



Analysis Technique



Systematic uncertainties: Accelerator

Accelerator: SuperKEKB	**Name** **Sample** **Source**	**Analysis**
Delivered Luminosity	Integrated Luminosity (Calibration) Link (Belle II measurement)	$\mathscr{B}(B^+ \to K^+ \nu \bar{\nu})$ Luminosity (NU)
***B*-dataset**	Number of BB (Calibration) Link (Belle II measurement)	$\mathscr{B}(B^+ \to K^+ \nu \bar{\nu})$

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Systematic uncertainties: Detector

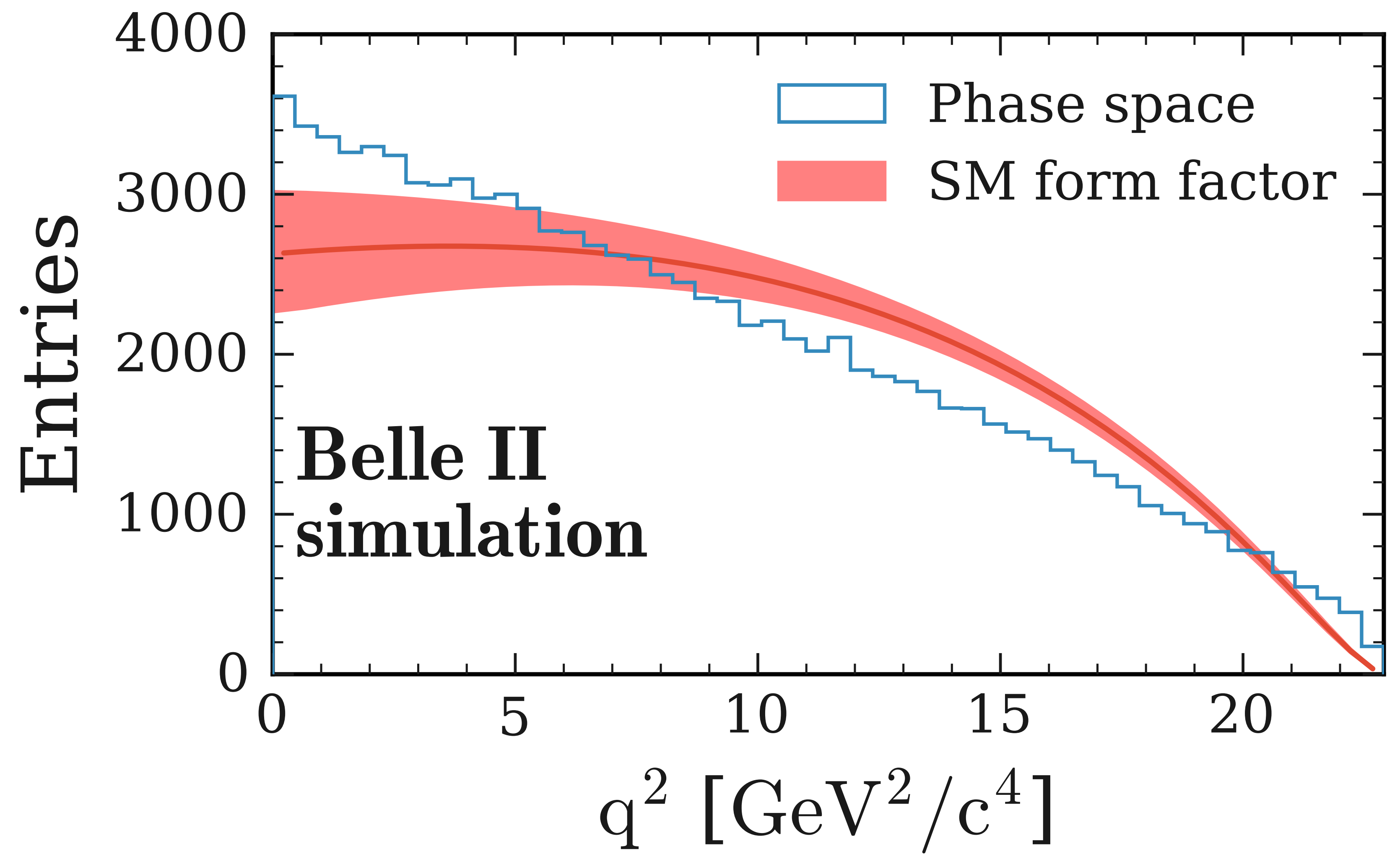
Detector and reconstruction: Belle II	Name Sample Source	Analysis Modifier
Tracking of charged particles	Tracking efficiency (Calibration) Belle II measurement ($e^+e^- \to \tau^+\tau^-$, link)	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Histosys
Measurement of energy deposit (photons)	Uncertainty on the absolute energy for photons (Calibration) Belle II measurement ($e^+e^- \to e^+e^-\gamma$, link)	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Histosys
Measurement of energy deposit (others)	Uncertainty on the absolute energy for other clusters (Calibration) PID sidebands	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Histosys
Particle Identification	Uncertainty on the PID corrections (Calibration) PID Systematics framework ($D^{*+}/J/\psi/K^0$, link)	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Histosys
K0L efficiency in ECL	Uncertainty on the K_L^0 correction (Calibration) $e^+e^- \to \phi\gamma$	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Histosys

Systematic uncertainties: Simulation

Simulation: Belle II	Name Sample Source	Analysis Modifier
Uncertainty on background BF	Uncertainty on the BF of leading B-background (Alternative simulation model) (Alternative simulation)	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Histosys
Background normalisation	Continuum background (Calibration) (Continuum/Off-resonance)	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Normsys
Alternative background template	$B^+ \to n\bar{n}K^+$ background (Alternative simulation model) (Alternative simulation)	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Histosys
Alternative background template II	$B \to D^0 \to K_L^0 X$ templates (Calibration) (PID sidebands)	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Histosys
MC statistical error		

Systematic uncertainties: Theory

Theory/ Signal Modelling	Name Sample Source	Analysis Modifier
Signal shape	Form Factor Uncertainty (Alternative theory (simulation) model) (link)	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Histosys
Signal efficiency	Signal efficiency (Embedded samples) $(B^+ \to J/\psi K^+)$	
Signal shape	Signal shape (Embedded samples) $(B^+ \to J/\psi K^+)$	



Systematic uncertainties: Further Analysis

Further Analysis	Name Sample Source	Analysis Modifier
Background shape	BDTc shape (Alternative models)	$\mathscr{B}(B^+ \to K^+\nu\bar{\nu})$ Histosys
Fitting bias	Fitting bias (Alternative models)	

Systematics uncertainties @ Belle II (pyhf x basf2)

Systematics due to lim. MC statistics (staterror)

We cannot generate infinite MC samples for signal and backgrounds:

- We have to take into account the uncertainty due to having limited MC statistics → staterror
- How do we calculate this with this for weighted Poissonian process?
  - Use $\sigma_{stat} = \sqrt{\sum_i (w_i^2)}$
  - See chapter 2 of this paper for more explanation (eq. 7)

Correlated systematics: Tracking (histosys)

Tracking inefficiency was measured with $e^+e^- \to \tau^+\tau^-$ channel (calibration) yielding 0.3%

- Produce alternative models for signal and backgrounds where we model this inefficiency:
  - We developed analysis-level tool:
    - **ModularAnalysis.removeTracksForTrackingEfficiencyCalculation (inputListNames, fraction, path=None))**

    Randomly remove tracks from the provided particle lists to estimate the tracking efficiency. Takes care of the duplicates, if any

    ◦

Correlated systematics: PID (histosys)

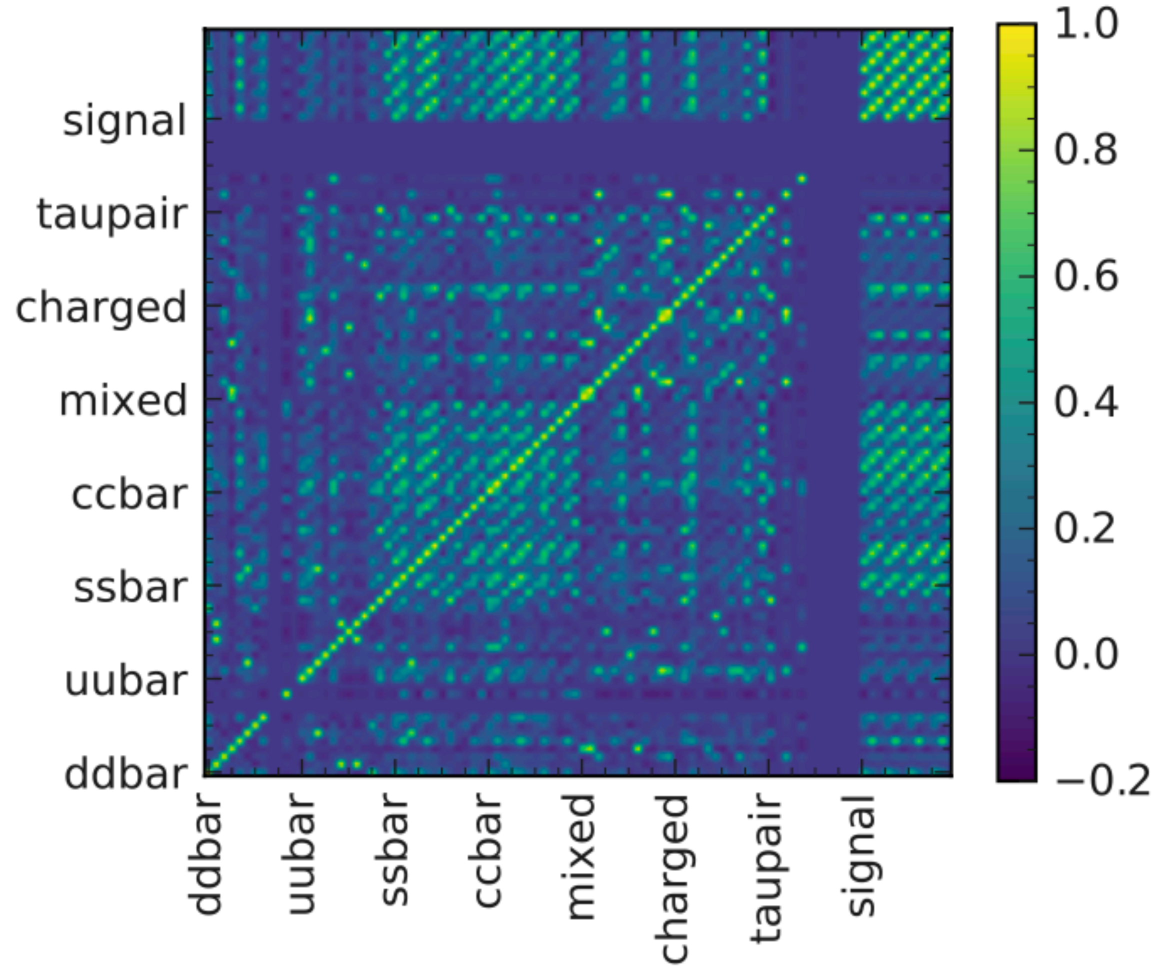
Method explained in [S.Glazov (Phystat 2021) p 7-9]

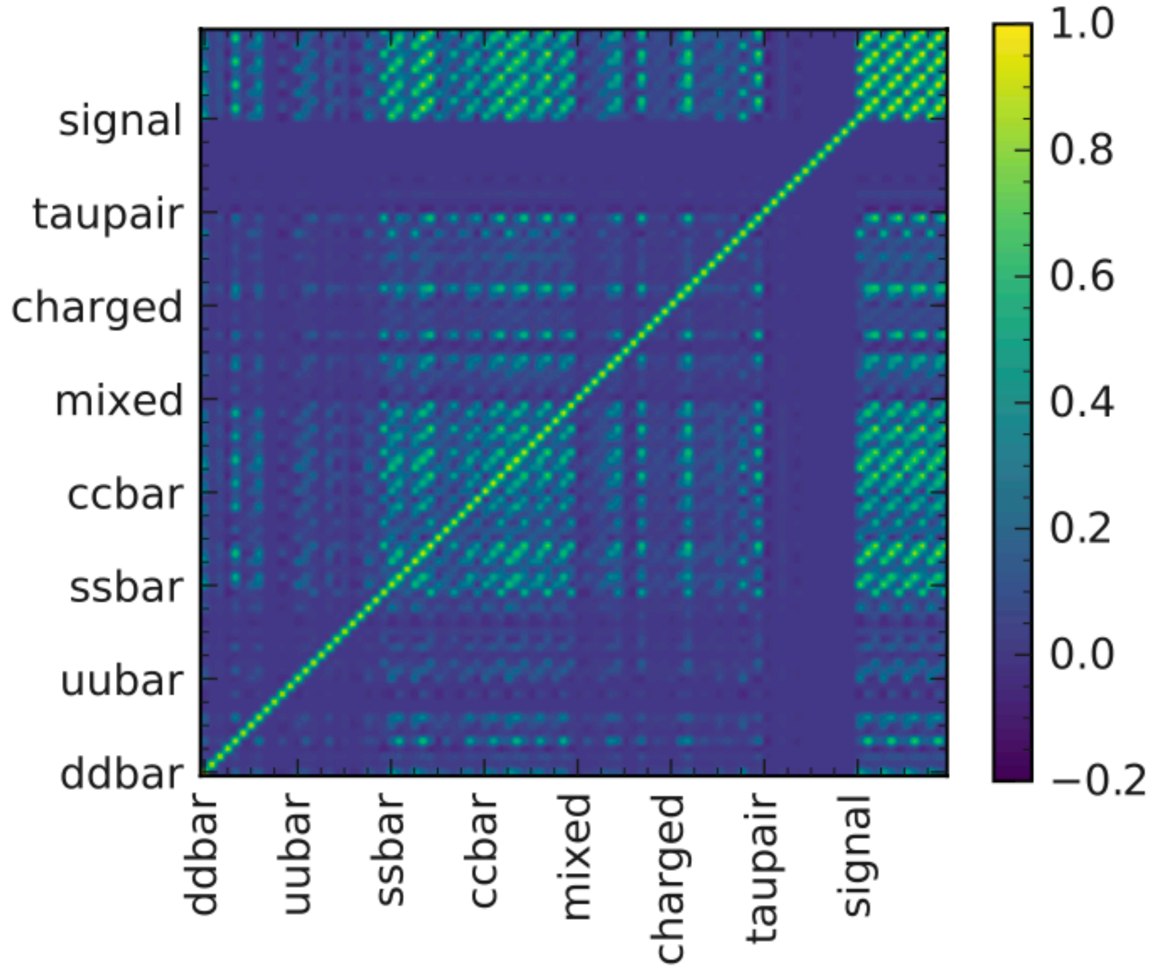
We use corrections from Systematics Framework to correct the kaon PID efficiency (weight)

- **These corrections are associated with uncertainty (PID), statistical error; σ:**
  - Non-trivial correlations PID corrections computed in bins of (p_T, θ)
  - Produce alternative simulations (toy MC): central values varied with lognormal$(0, \sigma)$
  - Construct covariance matrix
  - Translate to nuisance parameters: SVD decomposition + leading eigenvectors as the nuisances
    - More information can be found in Appendix N in the $B^+ \to K^+ \nu\bar{\nu}$ note
    -

$\mathscr{B}(B^+ \to K^+ \nu\bar{\nu})$

Full covariance





3 leading eigenvectors

Conclusion

In this lecture you have learnt:

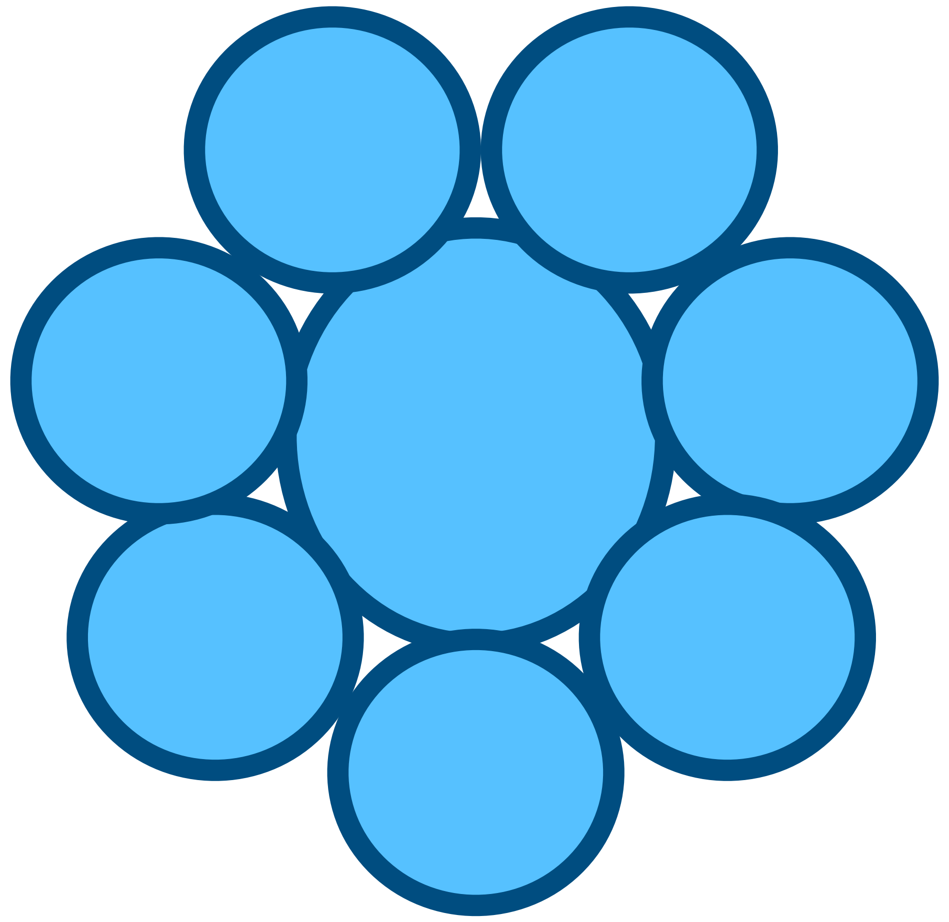
- When you can use pyhf
- How to build pyhf statistical model
- How to encode systematics into pyhf statistical model
- Where to find more information about HistFactory
- What kind of systematics you should worry about in Belle II
- What samples do you use for systematics uncertainties
- How do you calculate some of the most typical systematics

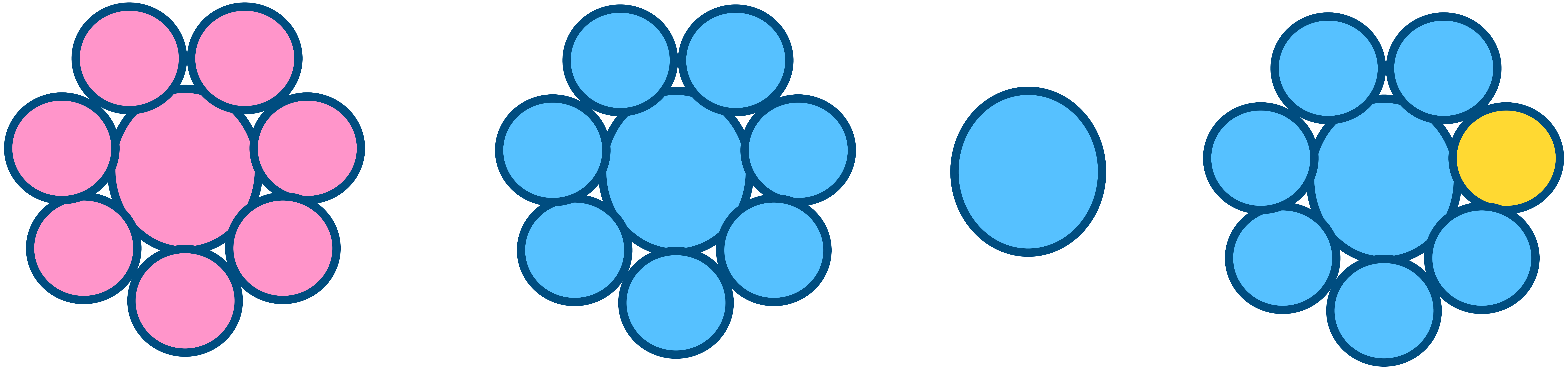
Please follow Lorenz's hands-on session for more!

Backup

When do we integrate systematics?

- When we know something in our analysis chain is maybe incorrect impacting on the measurement:
  1. Wrong → we apply corrections (known as calibrations)
  2. Uncertain → we do cross-checks:
     1. If passed with no major impact on the measurement → no action
     2. If major impact on the measurement → analysis is not robust
     3. If minor impact → **systematics and nuisance parameters**





Statistical model

[PRL 127, 181802 (2021)] ★

Set-up binned fit using HistFactory statistical model

- Likelihood based on HistFactory formalism implemented with pyhf + cross-check with sghf: simplified Gaussian model
  - Signal and background templates from MC
  - Separate templates for all backgrounds: mixed B, charged B, $c\bar{c}$, $u\bar{u}$, $s\bar{s}$, $d\bar{d}$, $\tau^-\tau^+$
  - All systematics included via nuisance parameters:
    - background normalisation uncertainty
    - tracking inefficiency
    - neutral energy mis-calibration for photons
    - neutral energy mis-calibration for unmatched photons
    - uncertainty on PID correction due to limited statistics
    - uncertainty on branching fractions of leading background processes
    - uncertainty on SM form factor
  - **Total number of fit parameters:**
    - 175 nuisance parameters ϕ
    - 1 parameter of interest (signal strength=μ)
    - **1 μ = SM $\mathscr{B}(B^+ \to K^+\nu\bar{\nu}) = (4.6 \pm 0.5) \times 10^{-6}$**

$$f(n, a \,|\, \eta, \chi) = \prod_{r \in \text{regions}} \prod_{b \in \text{bins}} \text{Pois}(n_{rb} \,|\, \nu_{rb}(\eta, \chi)) \prod_{\chi} c_\chi(a_\chi \,|\, \chi)$$

Simultaneous measurements of multiple regions

Constraints

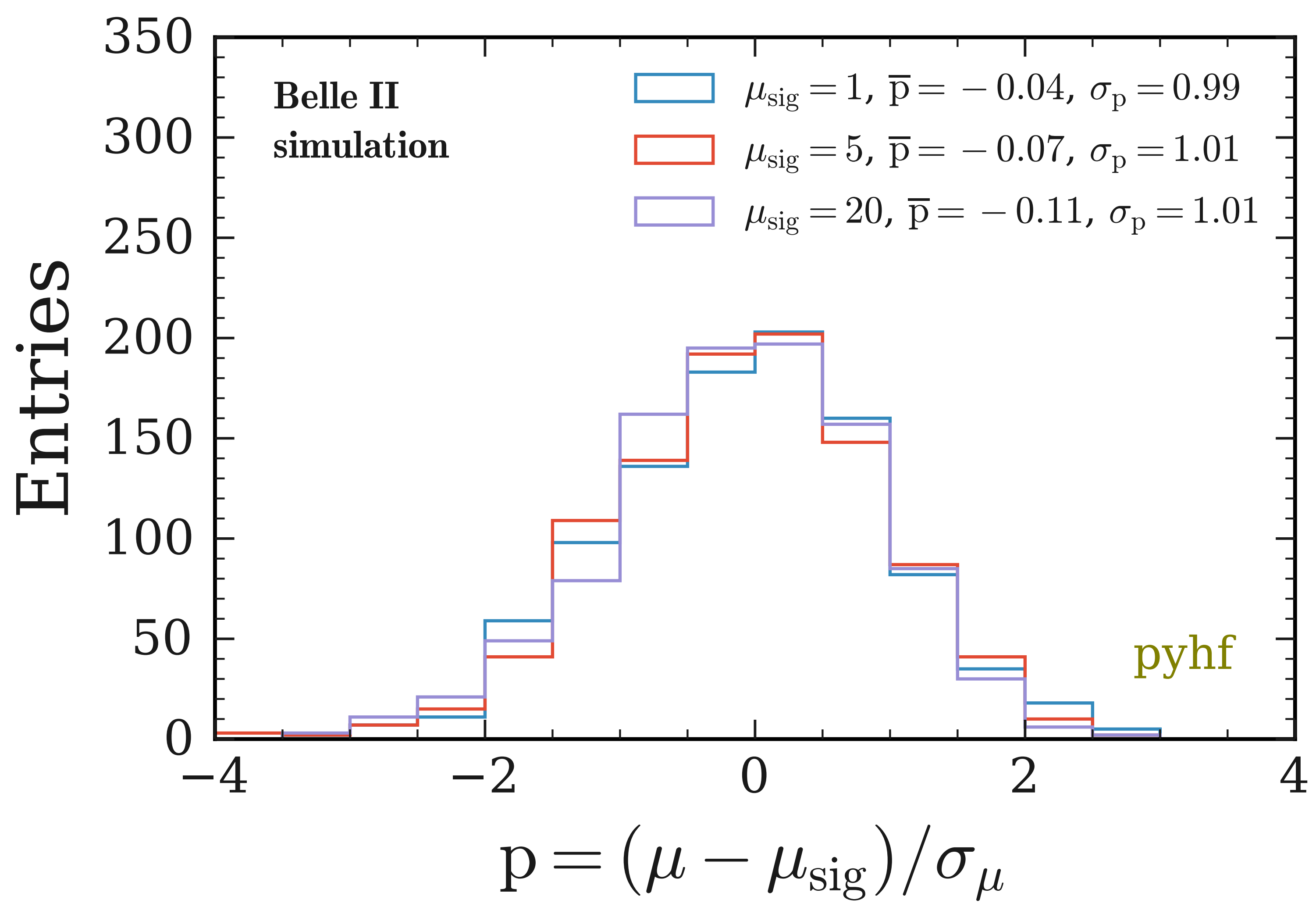
η = parameter of interest
χ = nuisance parameters

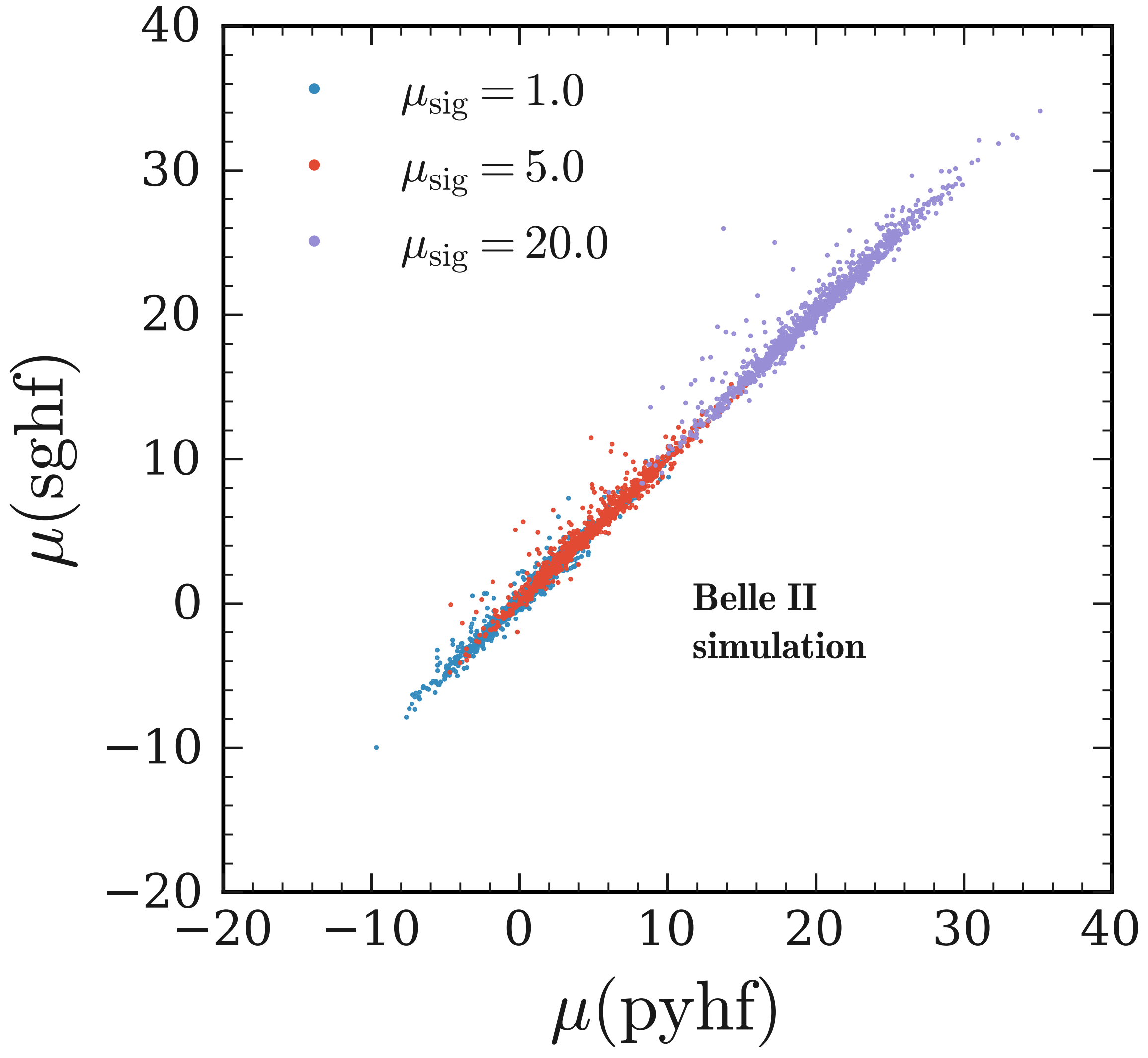
Fit validation

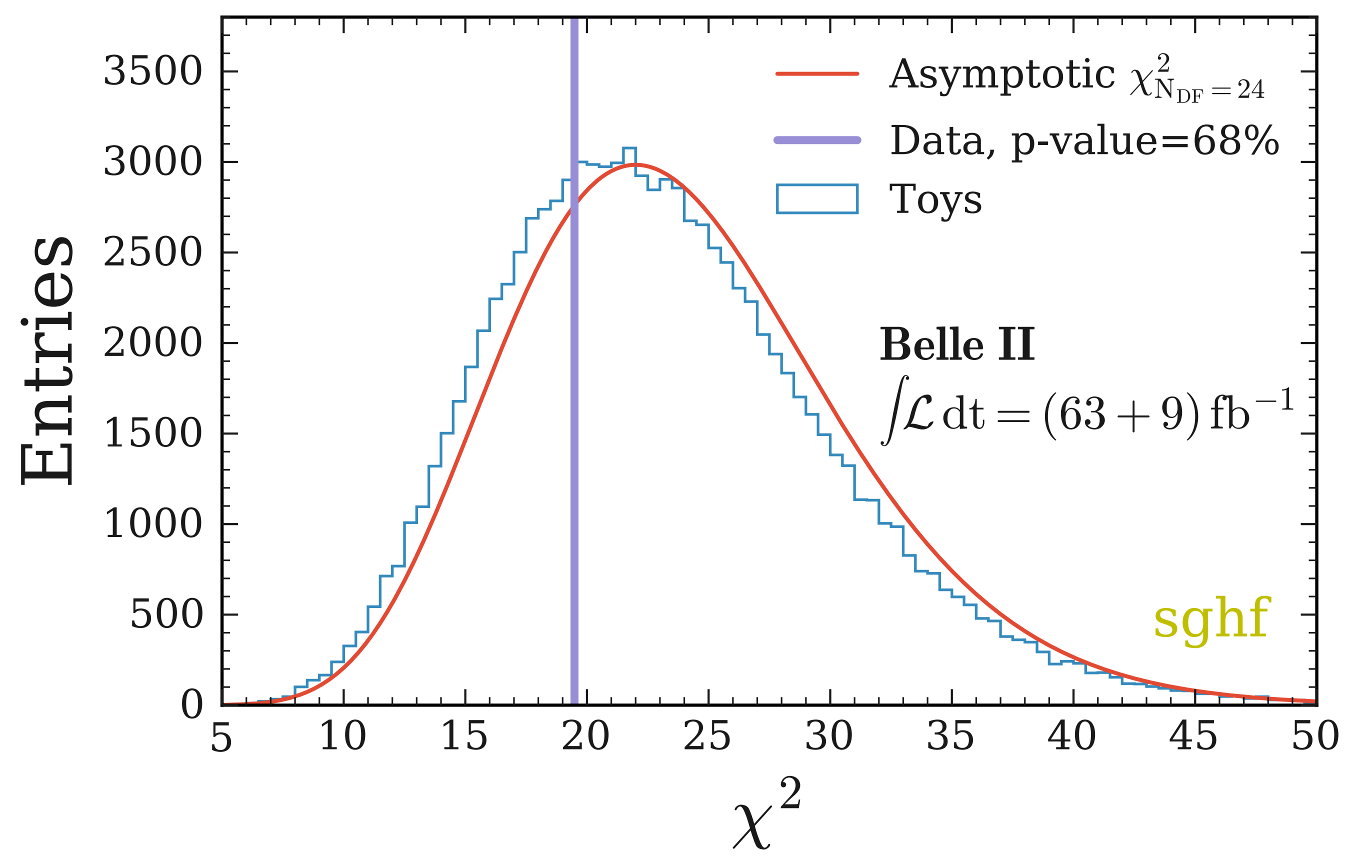
[PRL 127, 181802 (2021)] ★

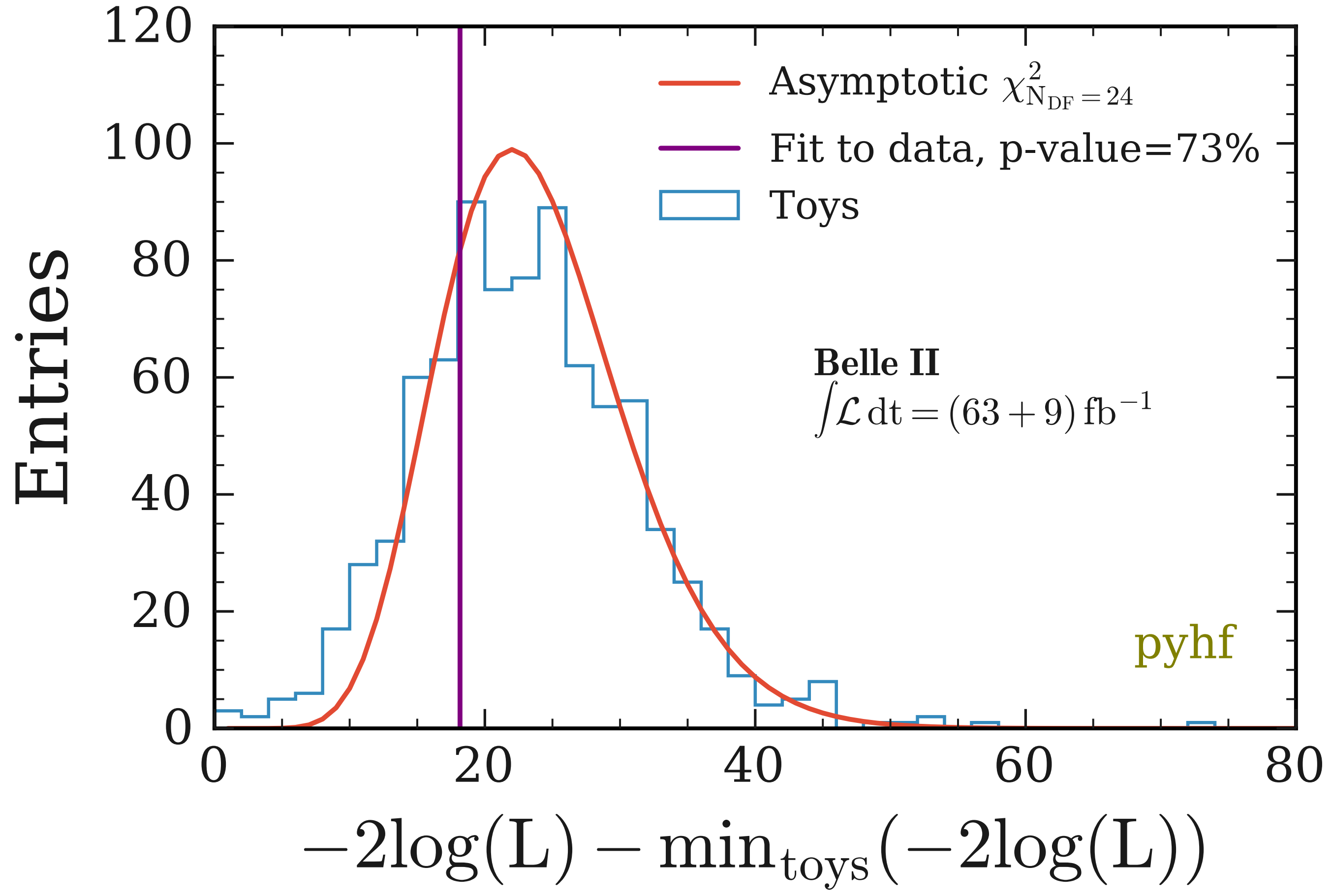
Perform Fit Bias Check

- Used because of high $\mathscr{B}$ and clean signature
- Generate toys with signal strength μ = 1, 5, 20 and check pulls = $\frac{\mu_{fit} - \mu_{inj}}{\sigma_\mu}$
- Results: 0 bias, expected μ recovered, very good agreement between pyhf and sghf









Check Data-Model Compatibility

- Generate toys and check fit quality
- Results: p-value shows good data model compatibility for both pyhf and sghf

What we learnt from fit? [PRL 127, 181802 (2021)]

1. $c\bar{c}$, $s\bar{s}$ continuum backgrounds are pulled up by 40%
2. Inclusive tag approach shows the best performance
    1. 3.5 better than HAD tag
    2. 20% better than SL Belle tag
    3. 10% better than HAD and SL tag
3. BSM $B^+ \to K^+\nu\bar{\nu}$ already with 1 ab^{-1}