Studies on Monte Carlo tuning using Bayesian analysis

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Motivation

- Monte Carlo (MC) simulations essential aspect of data analysis in HEP
- Parameters of parton shower and hadronisation models not derivable from first principles
  $\rightarrow$ Data driven methods
- Goal: Describe data as accurately as possible
- Applications in MC generators for air shower simulations

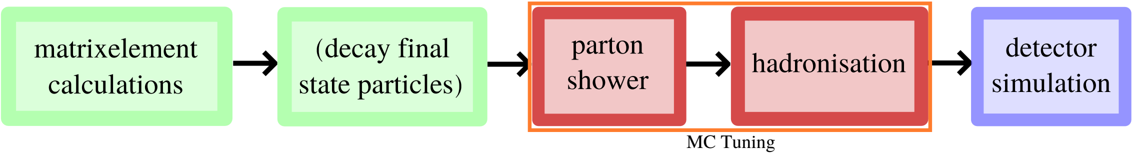


Figure: Graphical representation of MC event generation in collider experiments.

How to tune

- Multiple approaches (brute force, manually)
- Technical implementation can differ (mainly for the fits)
- State of the art: parametrization based tuning with Professor tool

(https://professor.hepforge.org/, arXiv:0907.2973)

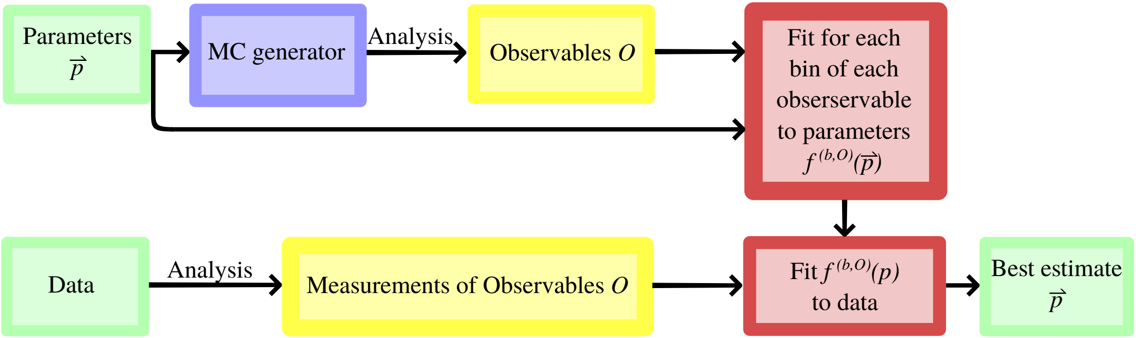


Figure: Schematic view of parameter based MC tuning.

MC Tuning using BAT

BAT.jl

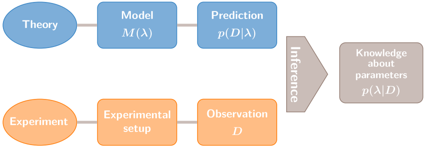
(https://github.com/bat/BAT.jl, arXiv:2008.03132)

- Rewrite of the Bayesian Analysis Toolkit in Julia
- Tool collection for statistical problems in a Bayesian context
- Numerical algorithms (such as MCMC) to explore posterior distributions

EFTfitter.jl

(https://github.com/tudo-physik-e4/EFTfitter.jl, arXiv:1605.05585)

- EFTfitter based on BAT.jl
- Generic tool build to interpret measurements in the context of EFT
- Applicable to any model to infer its parameters from data



Theory

Model $M(\lambda)$

Prediction $p(D|\lambda)$

Inference

Knowledge about parameters $p(\lambda|D)$

Experiment

Experimental setup

Observation D

MC Tuning in Julia

- Compatibility with Rivet histograms (similar to the Professor framework)
- Bin-wise-fit to MC possible with any user function
- Fit executed using LsqFit.jl package
  (https://github.com/JuliaNLSolvers/LsqFit.jl)
  - Least square fit with Levenberg-Marquardt minimization

- Fitting to data using BAT with the EFTfitter likelihood

$$-2\ln(\vec{p}|\vec{D}) = \sum_{i=1}^{n}\sum_{j=1}^{n}[\vec{D} - f^{(b,O)}(\vec{p})]_i \, M_{ij} \, [\vec{D} - f^{(b,O)}(\vec{p})]_j$$

- where M_{ij} is the covariance matrix between for each bin of each observable

Tuning Example

- Generated LEP events ($e^+ + e^- \to$ *jet jet* @ $\sqrt{s} = 91.2\,\mathrm{GeV}$) using `Herwig` at NLO
- RIVET (Robust Independent Validation of Experiment and Theory) (arXiv:1912.05451)
- Provides analysis code and data(!) for several example analyses + lightweight and fast

- Looking at event-shape variables, particle spectra and multiplicities
- Total about 100 histograms, with $\approx$ 1000 bins

Rivet and LEP example setup

- Parameters for cluster hadronisation in Herwig used for tuning
- 8 Parameters for tuning
  "AlphaQCD"
  "g:ConstituentMass (m(g))"
  "s:ConstituentMass (m(s))"
  "IRCutoff"
  "ClusterFissioner:ClMax"
  "ClusterFissioner:ClPow"
  "ClusterFissioner:PSplit"
  "ClusterDecayer:ClSmr"
- Parameters are varied from default values (50% up and down) (700 samples @ 1M events per sample)

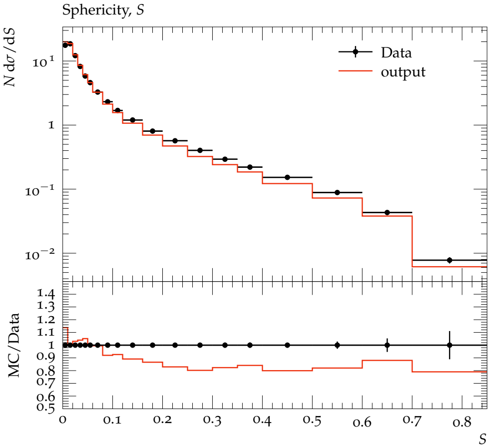
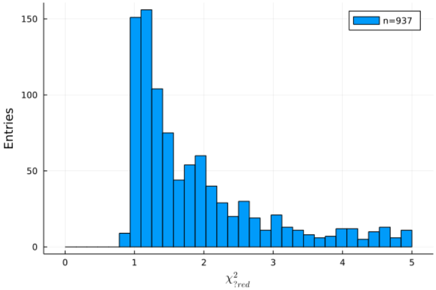
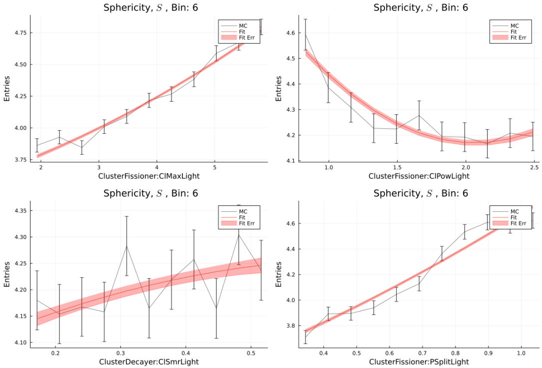


Figure: Sphericity using default tune values provided by Rivet.

Interpolation results

- Systematic find bad fits/low stat
- Reduced χ^2 and χ^2 probability as test statistics as goodness of fit
- Low p-values and/or high χ^2_{red} may indicate badly fitted bins/observables
  $\rightarrow$ Further look into those fits
- Bin-wise fit for first bins Sphericity for four parameters (on bottom)





Tuning Results

- BAT outputs distributions for parameters
- Marginalized 1D distributions shown for the first two parameters
- Next slide shows the correlation plots of all parameters

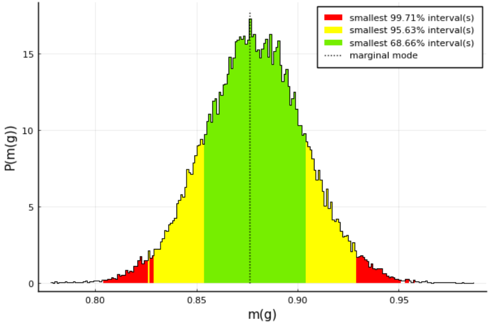


Figure: m(g),g:ConstituentMass

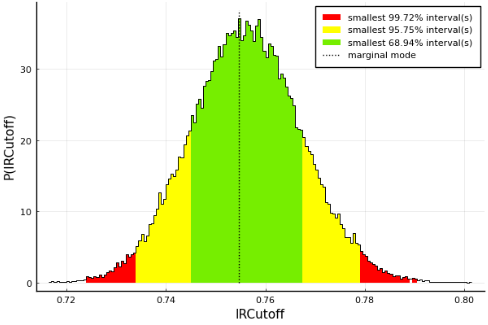
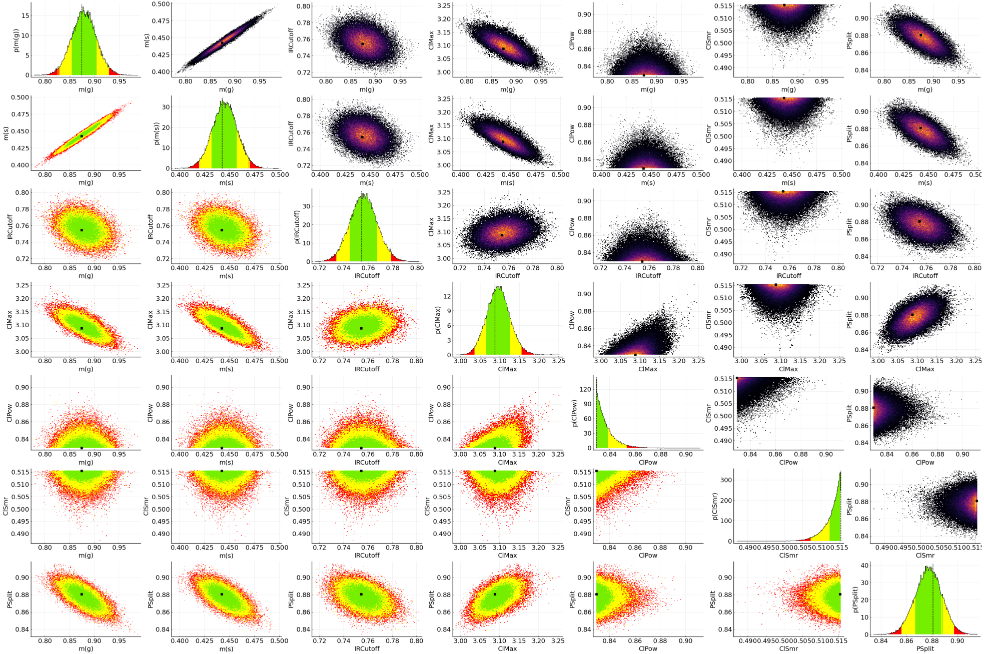
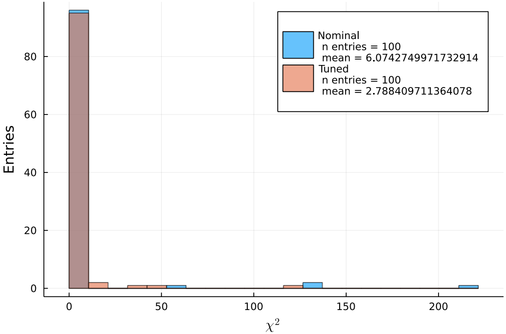
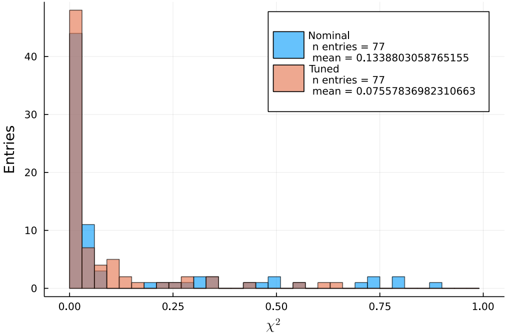


Figure: IRCutoff


p(m(g))
m(g)
0.80 0.85 0.90 0.95
p(m(s))
m(s)
0.400 0.425 0.450 0.475 0.500
p(IRCutoff)
IRCutoff
0.72 0.74 0.76 0.78 0.80
p(ClMax)
ClMax
3.00 3.05 3.10 3.15 3.20 3.25
p(ClPow)
ClPow
0.84 0.86 0.88 0.90
p(ClSmr)
ClSmr
0.490 0.495 0.500 0.505 0.510 0.515
p(PSplit)
PSplit
0.84 0.86 0.88 0.90

Tuning Results





- χ^2 values for data and MC for tuned and non-tuned values
- Right plot zoomed and cut values in between 0 and 1
- Visible reduction of χ^2 for tuned MC → better MC data agreement

Tuning in context of air showers simulations

- Air shower simulations show a significant muon deficit (muon puzzle)
- Most likely due to deviation of composition of secondary particles in hadronic interactions
- Further tuning of model parameters of air shower generators (possibly including LHC data)

- Compatibility-wise (what a tune needs):
  - MC generator with changeable parameters
  - A set of measurable observables (data)
  - Framework build in Julia, though at its core only needs histograms and parameters for MC and data
- Air shower MC generators such as EPOS or SIBYLL can be tuned
- SIBYLL already tuned with Professor (using RIVET)

Conclusion and Outlook

- Monte Carlo tuning using a Bayesian approach is possible/feasible
- Seamless integration of weighting for observables possible
- BAT tuning also allows for a straightforward implementation of correlated systematic uncertainties

- Studies on the effect on correlation and different weighting schemes towards the tuning results
- BAT tuning applicable to air shower/hadron interaction MC generators like SYBILL and EPOS
  → Future studies conducted by Michael Windau

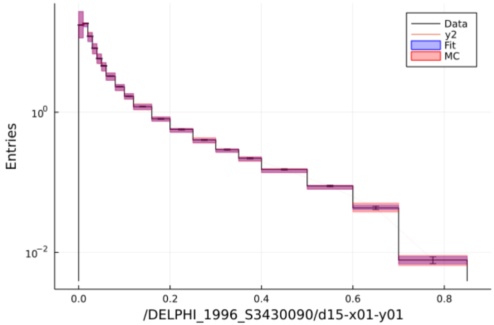
Thank you!

Backup

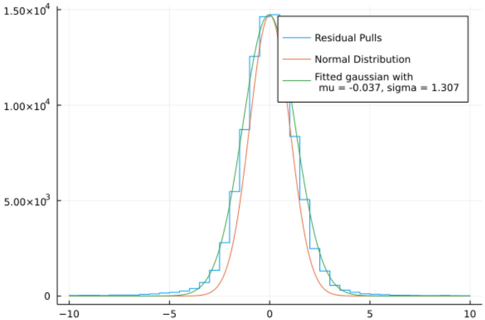
Full Observable List

Rivet analysis	code	clear text
ALEPH_1996_S3486095	d01-x01-y01	Sphericity, S (charged)
ALEPH_1996_S3486095	d02-x01-y01	Aplanarity, A (charged)
ALEPH_1996_S3486095	d03-x01-y01	1-Thrust, $1 - T$ (charged)
ALEPH_1996_S3486095	d04-x01-y01	Thrust minor, m (charged)
ALEPH_1996_S3486095	d07-x01-y01	C parameter (charged)
ALEPH_1996_S3486095	d08-x01-y01	Oblateness, $M - m$ (charged)
ALEPH_1996_S3486095	d09-x01-y01	Scaled momentum, $x_p = \|p\|/\|p_\text{beam}\|$ (charged)
ALEPH_1996_S3486095	d11-x01-y01	In-plane p_T in GeV w.r.t. sphericity axes (charged)
ALEPH_1996_S3486095	d12-x01-y01	Out-of-plane p_T in GeV w.r.t. sphericity axes (charged)
ALEPH_1996_S3486095	d17-x01-y01	Log of scaled momentum, $\log(1/x_p)$ (charged)
ALEPH_1996_S3486095	d18-x01-y01	Charged multiplicity distribution
ALEPH_1996_S3486095	d19-x01-y01	Mean charged multiplicity
ALEPH_1996_S3486095	d25-x01-y01	$\pi^\pm$ spectrum
ALEPH_1996_S3486095	d26-x01-y01	$K^\pm$ spectrum
ALEPH_1996_S3486095	d29-x01-y01	π^0 spectrum
ALEPH_1996_S3486095	d30-x01-y01	η spectrum
ALEPH_1996_S3486095	d31-x01-y01	η' spectrum
ALEPH_1996_S3486095	d32-x01-y01	K^0 spectrum
ALEPH_1996_S3486095	d33-x01-y01	Λ^0 spectrum
ALEPH_1996_S3486095	d34-x01-y01	Ξ^- spectrum
ALEPH_1996_S3486095	d35-x01-y01	$\Sigma^\pm(1385)$ spectrum
ALEPH_1996_S3486095	d36-x01-y01	$\Xi^0(1530)$ spectrum
ALEPH_1996_S3486095	d37-x01-y01	ρ spectrum
ALEPH_1996_S3486095	d38-x01-y01	$\omega(782)$ spectrum
ALEPH_1996_S3486095	d39-x01-y01	$K^{*0}(892)$ spectrum
ALEPH_1996_S3486095	d40-x01-y01	ϕ spectrum
ALEPH_1996_S3486095	d43-x01-y01	$K^{*\pm}(892)$ spectrum
ALEPH_2001_S4656318	d01-x01-y01	b quark fragmentation function $f(x_B^\text{weak})$
ALEPH_2001_S4656318	d07-x01-y01	Mean of b quark fragmentation function $f(x_B^\text{weak})$
DELPHI_1996_S3430090	d01-x01-y01	In-plane $p_\perp$ in GeV w.r.t. thrust axes
DELPHI_1996_S3430090	d02-x01-y01	Out-of-plane $p_\perp$ in GeV w.r.t. thrust axes
DELPHI_1996_S3430090	d03-x01-y01	In-plane $p_\perp$ in GeV w.r.t. sphericity axes
DELPHI_1996_S3430090	d04-x01-y01	Out-of-plane $p_\perp$ in GeV w.r.t. sphericity axes
DELPHI_1996_S3430090	d07-x01-y01	Scaled momentum, $x_p = \|p\|/\|p_\text{beam}\|$
DELPHI_1996_S3430090	d08-x01-y01	Log of scaled momentum, $\log(1/x_p)$
DELPHI_1996_S3430090	d09-x01-y01	Mean out-of-plane $p_\perp$ in GeV w.r.t. thrust axes vs. x_p
DELPHI_1996_S3430090	d10-x01-y01	Mean $p_\perp$ in GeV vs. x_p
DELPHI_1996_S3430090	d11-x01-y01	$1 -$ Thrust
DELPHI_1996_S3430090	d12-x01-y01	Thrust major, M
DELPHI_1996_S3430090	d13-x01-y01	Thrust minor, m
DELPHI_1996_S3430090	d14-x01-y01	Oblateness = $M - m$
DELPHI_1996_S3430090	d15-x01-y01	Sphericity, S
DELPHI_1996_S3430090	d16-x01-y01	Aplanarity, A
DELPHI_1996_S3430090	d17-x01-y01	Planarity, P
DELPHI_1996_S3430090	d18-x01-y01	C parameter
DELPHI_1996_S3430090	d19-x01-y01	D parameter
DELPHI_1996_S3430090	d33-x01-y01	Energy-energy correlation, EEC
DELPHI_1996_S3430090	d35-x01-y01	Mean charged multiplicity
JADE_OPAL_2000_S4300807	d26-x01-y01	Differential 2-jet rate with Durham algorithm (91.2 GeV)
JADE_OPAL_2000_S4300807	d26-x01-y02	Differential 3-jet rate with Durham algorithm (91.2 GeV)
JADE_OPAL_2000_S4300807	d26-x01-y03	Differential 4-jet rate with Durham algorithm (91.2 GeV)
JADE_OPAL_2000_S4300807	d26-x01-y04	Differential 5-jet rate with Durham algorithm (91.2 GeV)
PDG_HADRON_MULTIPLICITIES	d01-x01-y03	Mean π^+ multiplicity
PDG_HADRON_MULTIPLICITIES	d02-x01-y03	Mean π^0 multiplicity
PDG_HADRON_MULTIPLICITIES	d03-x01-y03	Mean K^+ multiplicity
PDG_HADRON_MULTIPLICITIES	d04-x01-y03	Mean K^0 multiplicity
PDG_HADRON_MULTIPLICITIES	d05-x01-y03	Mean η multiplicity
PDG_HADRON_MULTIPLICITIES	d06-x01-y03	Mean $\eta'(958)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d07-x01-y03	Mean D^+ multiplicity
PDG_HADRON_MULTIPLICITIES	d08-x01-y03	Mean D^0 multiplicity
PDG_HADRON_MULTIPLICITIES	d09-x01-y03	Mean D_s^+ multiplicity
PDG_HADRON_MULTIPLICITIES	d10-x01-y01	Mean B^+, B_d^0 multiplicity
PDG_HADRON_MULTIPLICITIES	d11-x01-y01	Mean B_u^+ multiplicity
PDG_HADRON_MULTIPLICITIES	d12-x01-y01	Mean B_s^0 multiplicity
PDG_HADRON_MULTIPLICITIES	d13-x01-y03	Mean $f_0(980)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d14-x01-y01	Mean $a_0^+(980)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d15-x01-y03	Mean $\rho^0(770)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d16-x01-y01	Mean $\rho^+(770)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d17-x01-y02	Mean $\omega(782)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d18-x01-y03	Mean $K^{*+}(892)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d19-x01-y03	Mean $K^{*0}(892)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d20-x01-y03	Mean $\phi(1020)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d21-x01-y03	Mean $D^{*+}(2010)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d23-x01-y02	Mean $D_s^{*+}(2112)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d24-x01-y01	Mean B^* multiplicity
PDG_HADRON_MULTIPLICITIES	d25-x01-y02	Mean $J/\psi(1S)$ multiplici
PDG_HADRON_MULTIPLICITIES	d26-x01-y01	Mean $\psi(2S)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d27-x01-y01	Mean $\Upsilon(1S)$ multiplicity
PDG_HADRON_MULTIPLICITIES	d28-x01-y01	Mean $f_1(1285)$ multiplici
PDG_HADRON_MULTIPLICITIES	d29-x01-y01	Mean $f_1(1420)$ multiplici
PDG_HADRON_MULTIPLICITIES	d30-x01-y01	Mean $\chi_{c1}(3510)$ multiplic
PDG_HADRON_MULTIPLICITIES	d31-x01-y03	Mean $f_2(1270)$ multiplici
PDG_HADRON_MULTIPLICITIES	d32-x01-y01	Mean $f_2'(1525)$ multiplici
PDG_HADRON_MULTIPLICITIES	d34-x01-y02	Mean $K_2^{*0}(1430)$ multiplic
PDG_HADRON_MULTIPLICITIES	d35-x01-y01	Mean B^{**} multiplicity
PDG_HADRON_MULTIPLICITIES	d36-x01-y01	Mean D_{s1}^+ multiplicity
PDG_HADRON_MULTIPLICITIES	d37-x01-y01	Mean D_{s2}^+ multiplicity
PDG_HADRON_MULTIPLICITIES	d38-x01-y03	Mean p multiplicity
PDG_HADRON_MULTIPLICITIES	d39-x01-y03	Mean Λ multiplicity
PDG_HADRON_MULTIPLICITIES	d40-x01-y02	Mean Σ^0 multiplicity
PDG_HADRON_MULTIPLICITIES	d41-x01-y01	Mean Σ^- multiplicity
PDG_HADRON_MULTIPLICITIES	d42-x01-y01	Mean Σ^+ multiplicity
PDG_HADRON_MULTIPLICITIES	d43-x01-y01	Mean $\Sigma^\pm$ multiplicity
PDG_HADRON_MULTIPLICITIES	d44-x01-y03	Mean Ξ^- multiplicity
PDG_HADRON_MULTIPLICITIES	d45-x01-y02	Mean $\Delta^{++}(1232)$ multipli
PDG_HADRON_MULTIPLICITIES	d46-x01-y03	Mean $\Sigma^-(1385)$ multiplic
PDG_HADRON_MULTIPLICITIES	d47-x01-y03	Mean $\Sigma^+(1385)$ multiplic
PDG_HADRON_MULTIPLICITIES	d48-x01-y03	Mean $\Sigma^\pm(1385)$ multiplic
PDG_HADRON_MULTIPLICITIES	d49-x01-y02	Mean $\Xi^0(1530)$ multiplic
PDG_HADRON_MULTIPLICITIES	d50-x01-y03	Mean Ω^- multiplicity
PDG_HADRON_MULTIPLICITIES	d51-x01-y03	Mean Λ_c^+ multiplicity
PDG_HADRON_MULTIPLICITIES	d52-x01-y01	Mean Λ_b^0 multiplicity
PDG_HADRON_MULTIPLICITIES	d54-x01-y02	Mean $\Lambda(1520)$ multiplicit

Other Interpolation tests

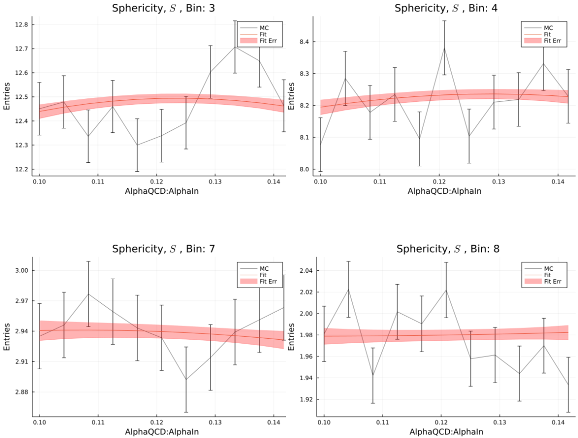


- Looking at maximum ranges of the fit vs MC (upper plot)
- Residual Pull plots using propagated fitting uncertainty (bottom plot)

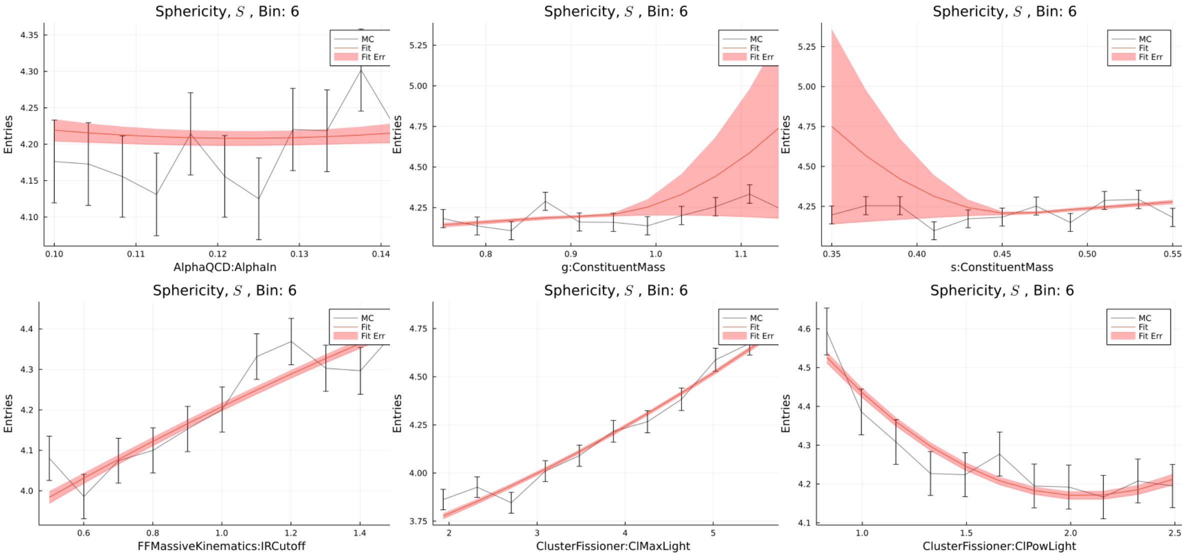


AlphaQCD Dependency

- There is no observed dependency on AlphaQCD in MC
- Matrixelement integration steps are performed beforehand to save on time which causes this effect

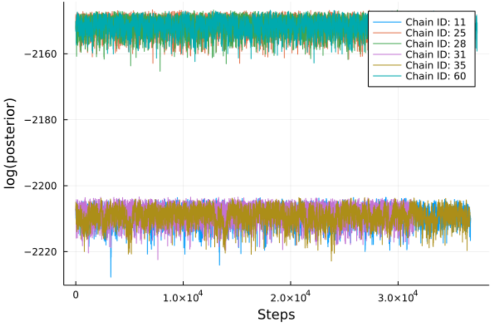


Interpolation rest

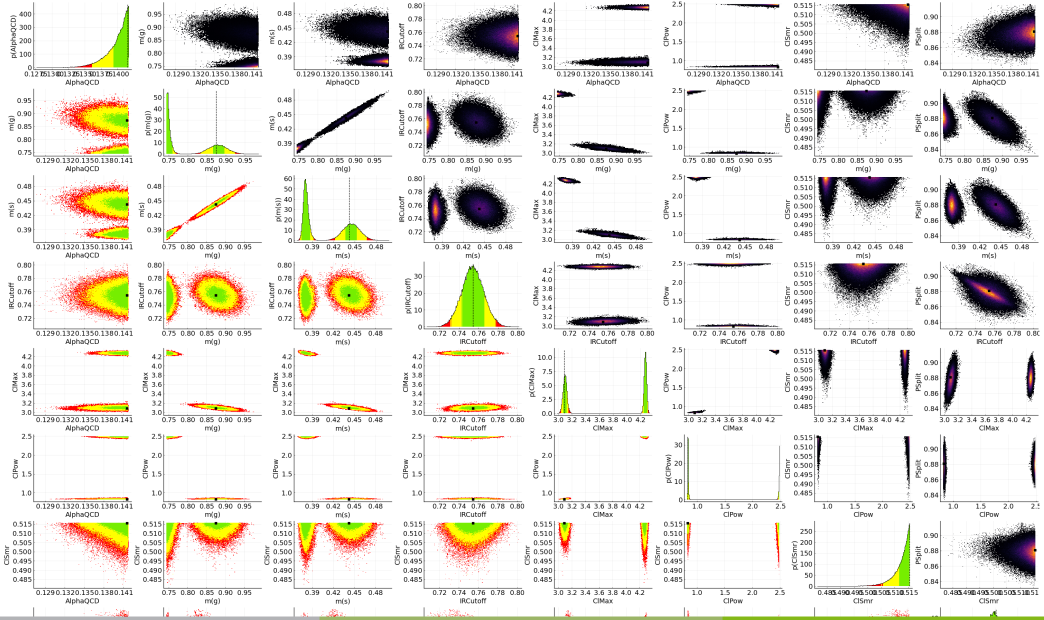


Removing MC Chains for secondary modes

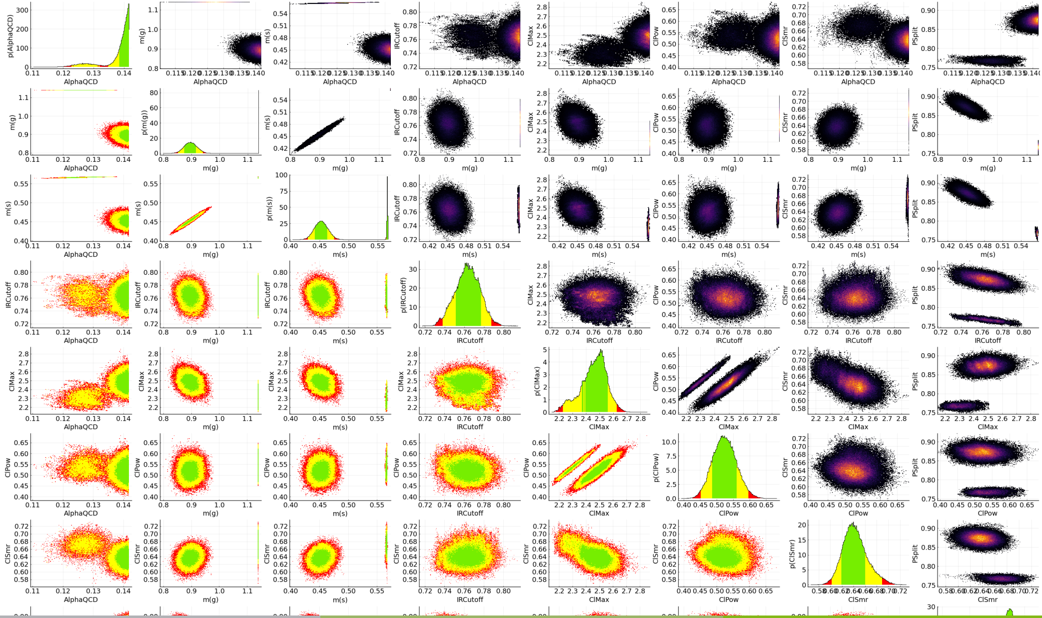
- Looking at the logposterior of the MC Chains (upper plot)
- Idea: Make Chains visible that get ’stuck’ in local small minima
- Remove those chains → re-run chains that found the global minimum



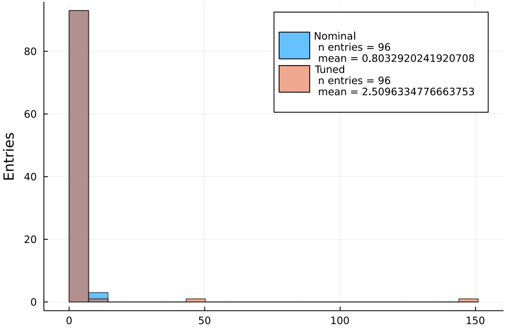
MC results with all chains

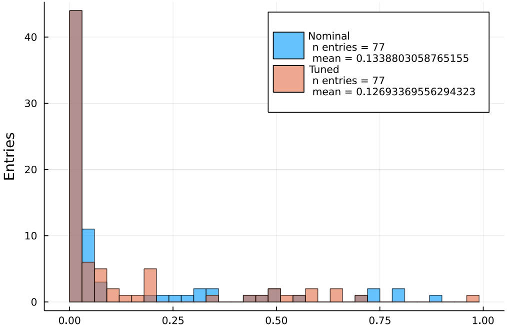


MC results with all chains and extrapolation



Tuning Results with extrapolation





- χ^2 values for data and MC for tuned and non-tuned values
- Right plot zoomed and cut values in between 0 and 1
- Visible reduction of χ^2 for tuned MC $\rightarrow$ better MC data agreement