

# Tuning a Monte Carlo Event Generator: Dos and Don'ts

Stefan Kiebacher in collaboration with Stefan Gieseke and Simon Plätzer | Non-Perturbative and Topological Aspects of QCD |  
May 28, 2024

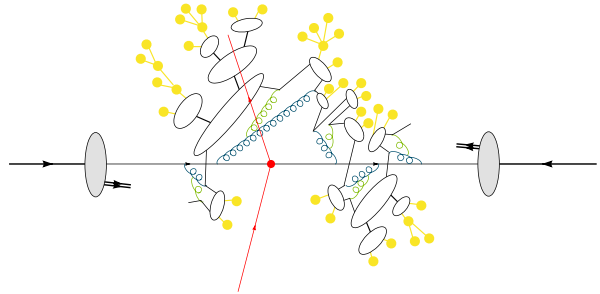
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Monte Carlo event generators:

- Simulation of high energy particle collisions
- Different codes such as Herwig, Sherpa and Pythia

Stages:

1. Hard Process (e.g. Drell-Yan  $pp \rightarrow e^+ e^-$ )
2. Parton Showers (initial and final state)
3. Hadronization
4. Colour Reconnection
5. Multiple Partonic Interactions (MPIs)



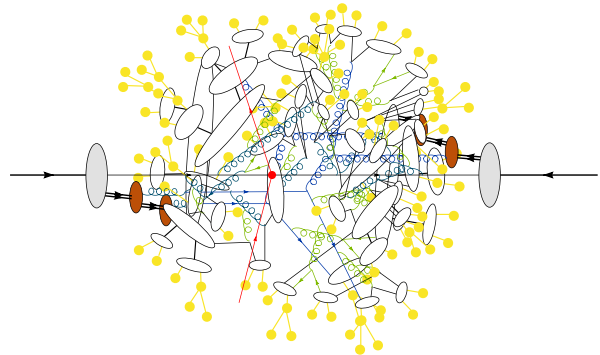
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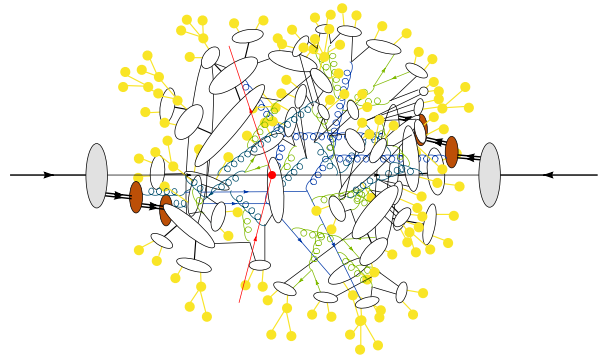
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⇒ Free parameters need to be "tuned"



# What is Tuning?

What is Tuning?

- Want the best description of the data without overfitting and without fitting away physics!  
⇒ Tuning
- Tuning essentially a glorified physics-informed fit to data (which data? which physics?)
- Compare new NP models/features to older models to assess the improvements
- **Not** for tuning a subset of data to better match the data! You might tune away physics and underestimate uncertainties

Talk will not be Minimum bias, but Herwig biased

- Will describe the typical data sensitive to each parts of NP modelling

# Minimum Bias Modelling Aspects

The most important building blocks for Minimum Bias (MB) modelling:

1. *Hadronization* (Should be universal, but is strongly connected to CR)
2. Colour Reconnection (CR)
3. Multiple Partonic Interactions (MPIs)
4. Diffraction
5. COM Energy evolution

# Hadronization

- Hadronization should be universal and is tuned to  $e^+ e^-$  data (LEP)
- Typically hadronization models have flavour parameters and flavour-blind parameters
- Flavour parameters make tune difficult  $\Rightarrow$  feedback with  $pp$  min bias tunes
- Choose (regions of) observables that your model can reasonably describe and are not dominated by pQCD (e.g. parton shower, hard process or multi-jet merging)!
- Choose parameters that are sensitive to the observables

# Hadronization

## Sensitive Observables:

- Event shapes peaks (e.g.  $T$ ,  $S$ ,  $D$ ,  $C$ , ...) [Hoang et al. 2024]
- Identified particle momentum spectra
- Multiplicities of (identified) hadrons

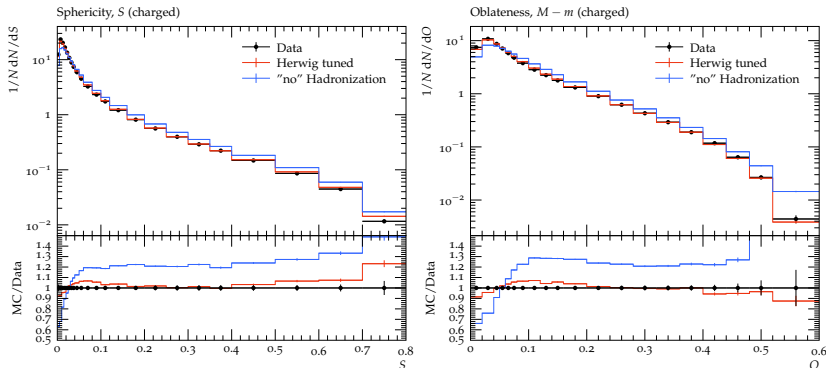


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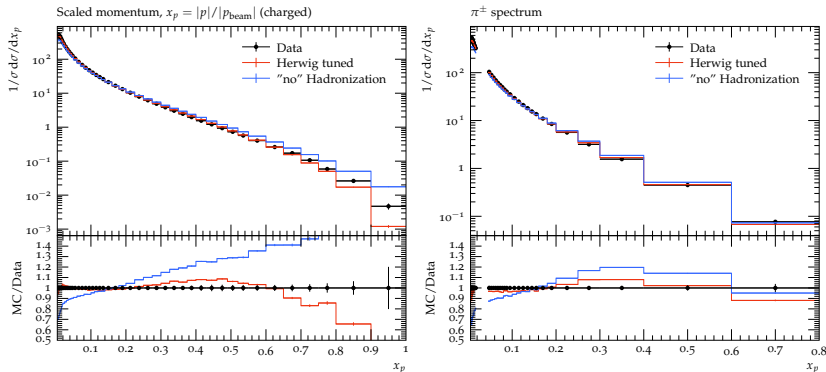


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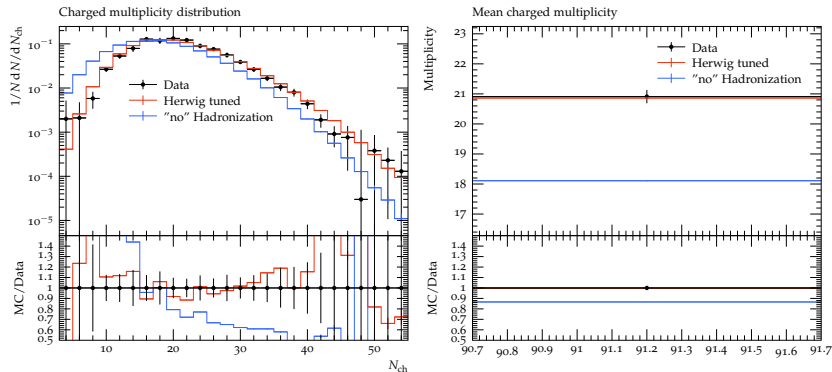


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# Colour Reconnection

- Colour Reconnection (CR) has little (but non-zero) impact at  $e^+e^-$  data
- If baryons can be formed in the CR model this will impact baryons multiplicities and momenta at  $e^+e^-$  data!  $\Rightarrow$  Might need to tune CR also to some extent to  $e^+e^-$  data
- Often CR is only tuned to minimum bias data
- CR generically reduces multiplicities and increases the  $\langle p_T \rangle(N_{\text{ch}})$  (if MPIs are active)
- CR and MPI variations also impacting VBS/VBF topologies [Bittrich et al. 2022]

# Colour Reconnection

## Sensitive Observables:

- Prime example of CR  
 $\langle p_T \rangle (N_{ch})$
- Multiplicity distributions in  $\eta, p_T$  (also for identified hadrons) for different MB cuts  
 $\Rightarrow$  might have feedback with hadronization flavour parameters

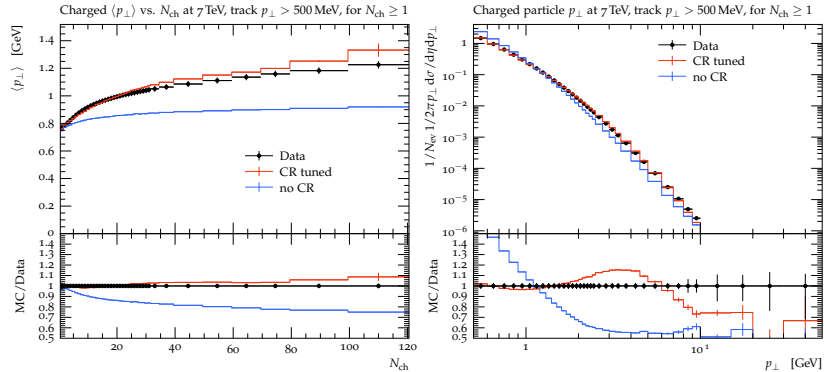


Figure: ATLAS and ALICE data [G. Aad et al. 2011] [Adam et al. 2015]

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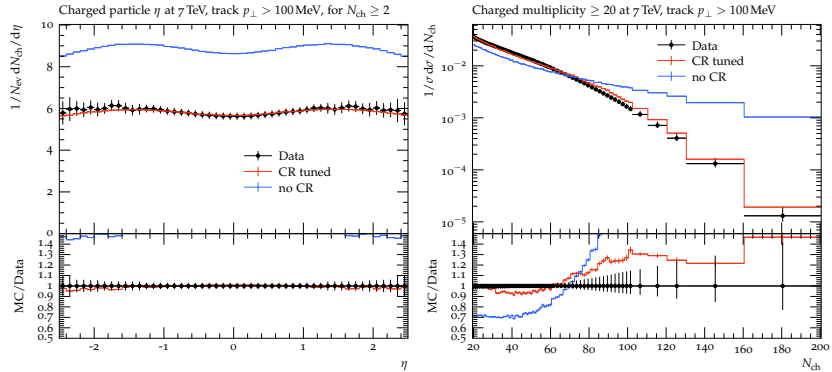


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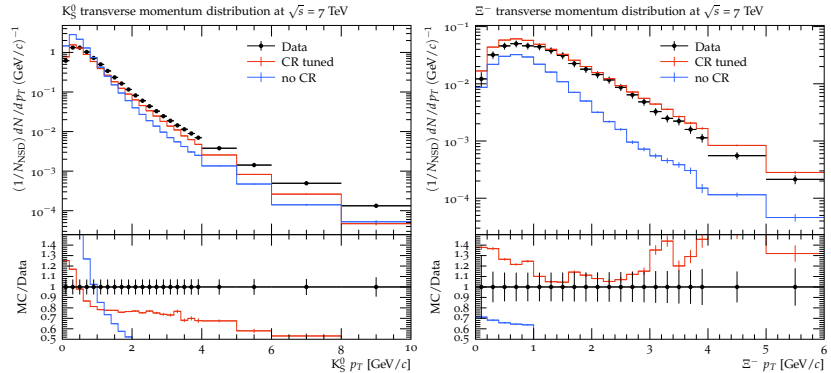


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# Multiple Partonic Interactions (MPIs)

- MPIs have no impact at  $e^+e^-$  data  $\Rightarrow$  only tune to  $pp$  and  $p\bar{p}$  MB data
- Can use  $\langle p_T \rangle(p_T^{\text{jet}})$ ,  $\langle N_{\text{ch}} \rangle(p_T^{\text{jet}})$  as cross check for MB tune
- In Herwig's eikonal model only 3 free parameters
- MPIs mostly affect multiplicities,  $p_T$  spectra and everything related to those.
- Should be mostly flavour-blind, but is strongly correlated to CR, which may impact flavours

# Multiple Partonic Interactions (MPIs)

Sensitive Observables:

- Multiplicity distributions
- Multiplicity in  $\eta$ ,  $p_T$  for different MB cuts

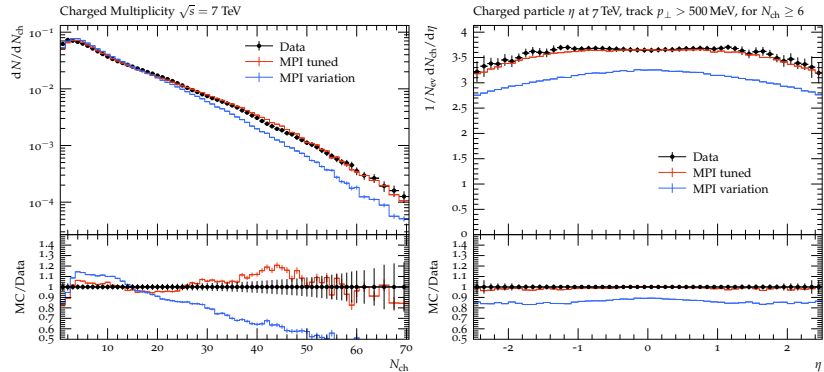


Figure: ATLAS and ALICE data [Aamodt et al. 2010], [G. Aad et al. 2011], [Georges Aad et al. 2011]



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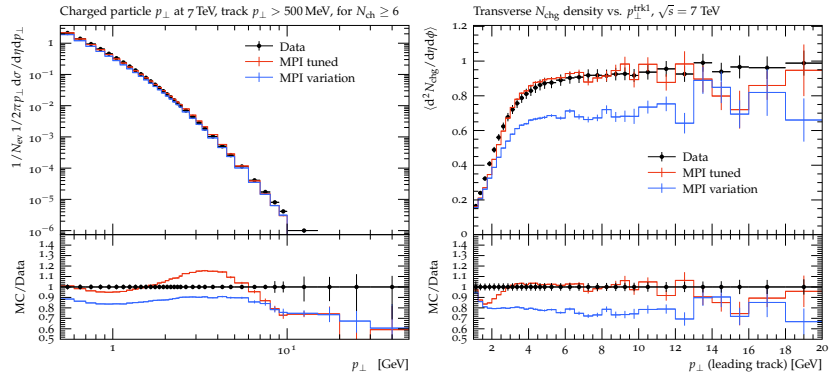


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# Diffraction

- Diffraction has very forward, low multiplicity signatures

Sensitive Observables:

- Prime example of Diffraction: Large rapidity gap  $\Delta\eta_L$
- Low multiplicity observables e.g. with very inclusive MB cuts

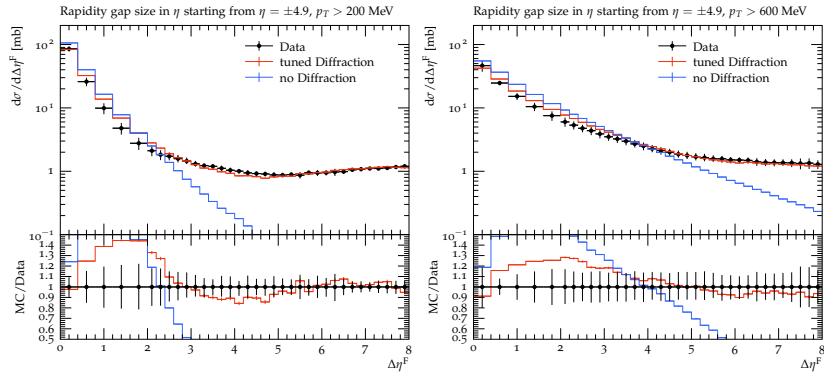


Figure: ATLAS data [Georges Aad et al. 2012]

# COM Energy evolution

- Standard MB tunes are tuned for a various selection of COM energies  $\sqrt{s} \in \{200, 500, 900, 1800, 7000\}$  GeV  
 [Bellm, Gieseke, and Kirchgaesser 2020]
- In Herwig  $p_T^{\min}(\sqrt{s})$  power law dependence of the parameters, by fit evolution to tune for each energy
- New Herwig MB tunes currently in progress (released with Herwig 7.4.0)

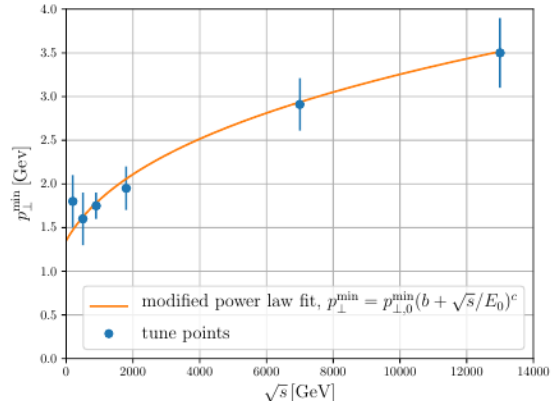


Figure: [Bellm, Gieseke, and Kirchgaesser 2020]

# Money Plots

Hadronization Model Tune:

- Improved hadronization model [Hoang et al. 2024] [Plätzer 2023]

String Model Tune for Herwig:

- String model plugin (preliminary tune)

[Sarmah et al. 2024]

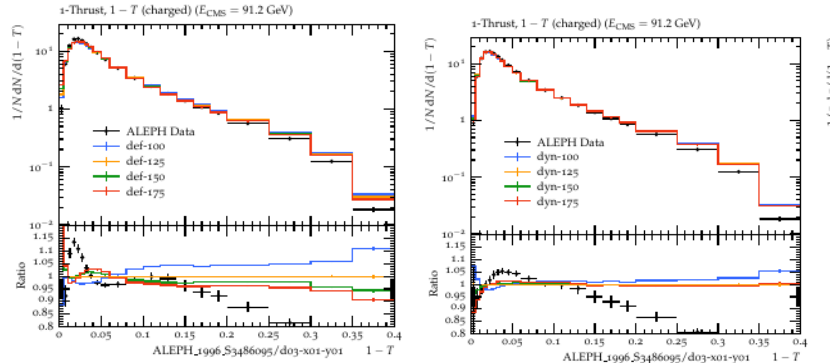


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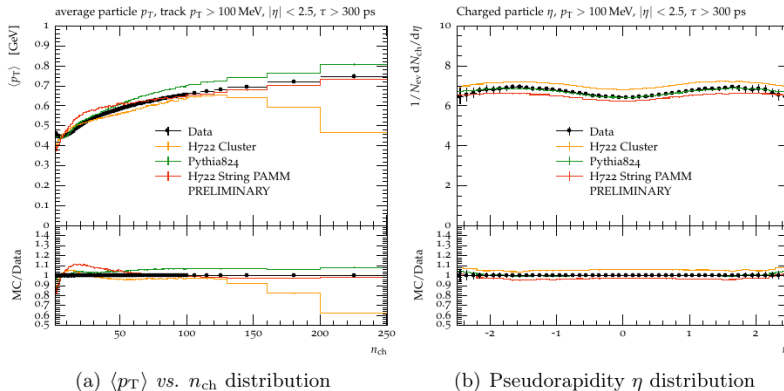


Figure: ATLAS data [Aaboud et al. 2016] [Aaboud et al. 2017]

# Tools

Lots of automatised tuning tools out there:

- Professor [Buckley et al. 2010]
- Apprentice [Krishnamoorthy et al. 2021]
- AutoTunes [Bellm and Gellersen 2020]
- Event generator tuning using Bayesian optimization [Ilten, Williams, and Yang 2017]
- Reweighting of hadronization parameters [Christan Bierlich et al. 2023]

The first 3 are based on the same principle:

- Sample the parameter space and run your event generator on those samples on a lot of data
- Interpolate all data bins of the samples using a (rational) polynomial (always verify that the interpolation is faithful!)
- Minimize a loss function according to some set of weights (always provide the weight files!)

# Professor

Tried and tested Professor has many features:

- Allows for polynomial interpolation of the data  $f_b(\vec{p}) = \alpha_b + \sum_i \beta_{b,i} p_i + \sum_{i,j} \gamma_{b,ij} p_i p_j + \dots$
- Loss function  $\chi^2(\vec{p}) = \sum_b w_b \frac{(f_b(\vec{p}) - \text{data}_b)^2}{\sigma_{b,\text{data}}^2 + \sigma_{b,\text{stat}}^2} \equiv \sum_b w_b \chi_b^2(\vec{p})$
- Build-in feature of dividing up samples into subsets and tune individually (for more robust tunes)

New features:

- Percentage "theory" error to avoid overfitting  $\sigma_{b,\text{theory}} = \lambda \cdot \text{data}_b$ , where  $\lambda \in [0, 1)$  and typically  $\lambda \sim 3 - 10\%$
- New regularized loss functions to avoid fitting bins that the model cannot describe (thanks to James Whitehead for the idea) e.g.  $\chi_{\text{reg}}^2(\vec{p}) = \sum_b w_b \frac{\chi_b^2(\vec{p})}{1 + \chi_b^2(\vec{p})}$

Downsides:

- Only polynomial interpolation
- No automatic weight selection nor bin rejection (if the bin cannot be described)
- Relatively slow
- Can only handle  $\lesssim 10$  parameters

# Apprentice

Apprentice is essentially a rewrite of Professor with new features:

- Allows for rational polynomial interpolation of the data  $f_b(\vec{p}) = \frac{p_b(\vec{p})}{q_b(\vec{p})}$  of order  $(m, n)$
- Build-in bin rejection if the envelope of the samples cannot describe a bin, it is ignored
- Faster than Professor
- Has bilevel optimization, which adaptively select weights

Downsides:

- Some features of Professor are missing
- Not supported anymore? work in progress by Stephen Mrenna
- Can only handle  $\lesssim 10$  parameters



# AutoTunes

AutoTunes is using Professor and extends it to handle more parameters

- Breaks down parameter space into minimally correlated subspaces and iteratively tunes those subspaces
- Can handle many parameter

Downsides:

- Setup tricky
- Need to give subdivisions (cannot have prime number of parameters)
- In each iteration a explorative tune on the full space needs to be performed
- Not supported anymore

# Data Selection and Weighting

Data quality requirements:

- Decent statistics in data and in event generator
- Most finegrained bins, without compromise on statistics are preferred
- No holes in histograms
- Prefer regular histograms instead of ratios of histograms (controversial, but IMO  $\frac{\text{garbage1}}{\text{garbage2}} \stackrel{?}{=} \text{good}$ )
- No double counting (or account for it) same observables measured by different experiment (just take the best) Call for benchmark weight sets!

Weight selection:

- Weights still have to put in by hand and no clear guideline on how to do this
- There are no benchmark weights sets which allow us to reasonably compare the performance of two event generators

# Wishlist: Tuning Targets

- We need better Rivet coverage especially for  $pp$  of ALICE!  
<https://rivet.hepforge.org/rivet-coverage> [Christian Bierlich et al. 2020]
- More identified particle spectra for MB binned in multiplicities
- Identified  $\langle p_T \rangle(N_{\text{ch}})$  (baryons and mesons)
- More statistics for high **and** low energy  $e^+e^-$  collisions to nail down hadronization tunes (especially to be ready for the next collider  $e^+e^-$  collider)
- More correlation data if the statistics are sufficient

# Status and Summary

## Status:

- Herwig 7.3.0 is out with new hadronization tunes, but no new MB tunes [Bewick et al. 2023]
- Herwig 7.4.0 will come with new MB tunes






## Summary:

- Tuning is not just an straightforward optimization problem
- Both expert manual tunes and automatised tools are somewhat biased
- In both cases human bias needs to select weights
- Opinion: Automatised tools used by an expert are preferred as they are reproducible and take less time
- Call to action on releasing Rivet analyses with your analyses
- Do not tune brute force without knowing what you might mess up, just to fit to data better!







Thank You For Your Attention!

Questions? Remarks? Comments?








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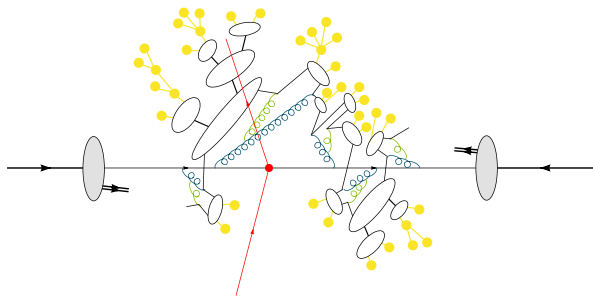
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# Introduction to Monte Carlo Event Generators

Stages of hadronization model in Herwig:

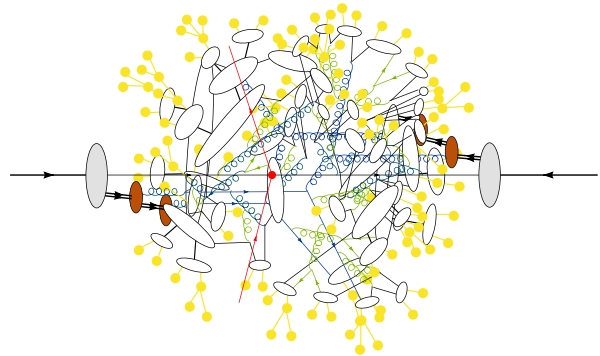
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- Primordial cluster formation
- Colour Reconnection (CR)
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# What is tuning? AI version

- Ask Chat GPT (3.5):

*What is the best strategy for tuning a general purpose monte carlo event generator like Herwig, Pythia or Sherpa?*

## ChatGPT

Tuning a Monte Carlo event generator like Herwig, Pythia, or Sherpa involves adjusting various parameters to match experimental data as closely as possible. Here's a general strategy for tuning such generators:

1. **Understand the Physics:** Before starting the tuning process, ensure a thorough understanding of the physics underlying the event generator. This includes the processes being simulated, the kinematics involved, and the relevant theoretical frameworks.
2. **Select Experimental Data:** Identify experimental data sets that are relevant to the processes you want to simulate. This could include measurements of cross-sections, particle distributions, event topologies, etc. Ensure that the data sets cover a wide range of energies and processes to provide a comprehensive test for the generator.
3. **Define Performance Metrics:** Establish quantitative metrics to assess the agreement between the generator predictions and the experimental data. These metrics could include chi-squared values, ratios of cross-sections, or various distributions.

# What is tuning? AI version

## ChatGPT

1. **Initial Parameter Setup:** Start with the default or commonly used parameter settings provided by the generator. This serves as a baseline for further tuning.
2. **Systematic Parameter Variation:** Systematically vary the parameters of the event generator and generate simulated events for each set of parameters. Parameters to be tuned may include particle masses, coupling constants, parton distribution functions (PDFs), fragmentation functions, etc. It's essential to understand the impact of each parameter on the generated events.
3. **Compare with Experimental Data:** Compare the simulated events with the experimental data using the established performance metrics. Identify regions where the agreement is good and areas where improvements are needed.
4. **Iterative Optimization:** Use optimization algorithms or manual adjustments to iteratively improve the agreement between the simulated events and the experimental data. This involves fine-tuning the parameters to minimize the discrepancies.

# What is tuning? AI version

## ChatGPT

1. **Validation:** After each round of tuning, validate the tuned parameters by comparing the predictions with independent experimental data sets that were not used in the tuning process. This helps ensure that the tuning procedure does not lead to overfitting.
2. **Documentation and Analysis:** Document the tuned parameter sets and the corresponding agreement with experimental data. Analyze the impact of each parameter on the generator's performance and understand any remaining discrepancies.
3. **Community Feedback:** Share the tuned parameter sets and results with the community working on similar physics processes. Collaborate with experimentalists and theorists to further validate the tuned generator and improve its accuracy.
4. **Continual Improvement:** The tuning process is ongoing as new experimental data becomes available or as theoretical understanding advances. Regularly revisit the tuning procedure to incorporate new information and improve the accuracy of the event generator.

By following these steps and employing a combination of physics knowledge, computational techniques, and experimental data analysis, one can effectively tune a Monte Carlo event generator to accurately simulate a wide range of particle physics processes.