MC Tuning

Judith Katzy (DESY)

- MC Tuning of phenomenological models: the methods
- MC comparisons to data (Unfolding)
- Tuning of specific parameters with sensitive observables
- Tuning of matched generators

Motivation for MC tuning

MC generators important tools to

- Derive resolution and accepetance corrections
- Estimate backgrounds
- Design detectors
- Provide theoretical interpretation of the results

➢ Need good description of ALL aspects of high energy interaction

- differential distributions of final state objects like jets and leptons produced in either the hard process or additional physics processes

➢ Check and tune models with available data

"The experience gained with the model, in failures as well as successes, could be used as a guideline in the evolution of yet more detailed models." [T.Sjoestrand, 1987]

Observables and the partonic picture

Hard interactions

Jets
Leptons

Radiation effects

Inner jet structure
Small angle lepton distributions

Soft QCD

Soft charged particles
Energy flow

Short distance physics
- Small α_s
- Perturbative calculations

Factorisation

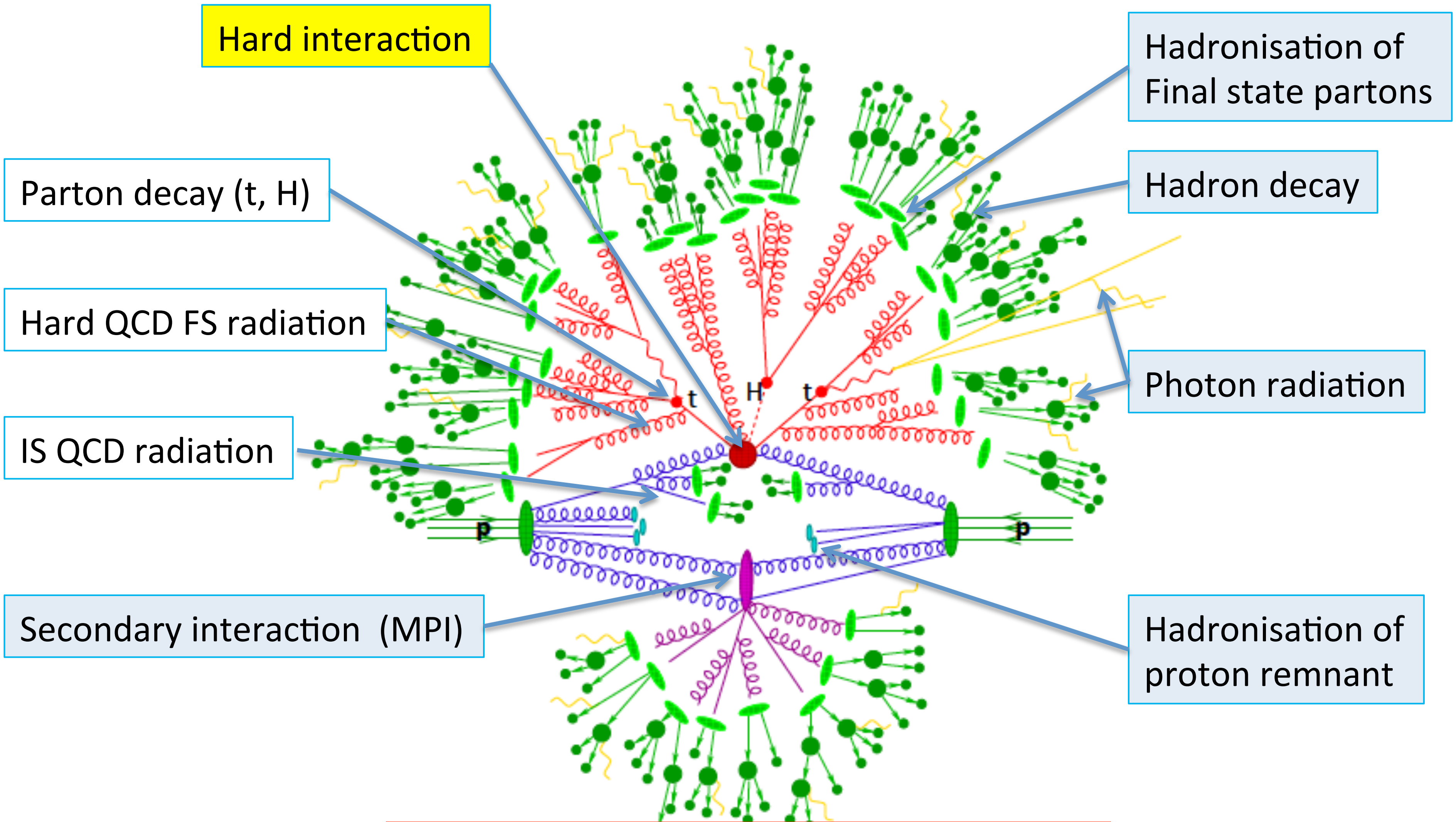
Large distance physics
- Large α_s
- Phenomenological models
- Universality

Universality of phenomenological models

Underlying assumption: non-perturbative dynamics independent of the hard scattering process

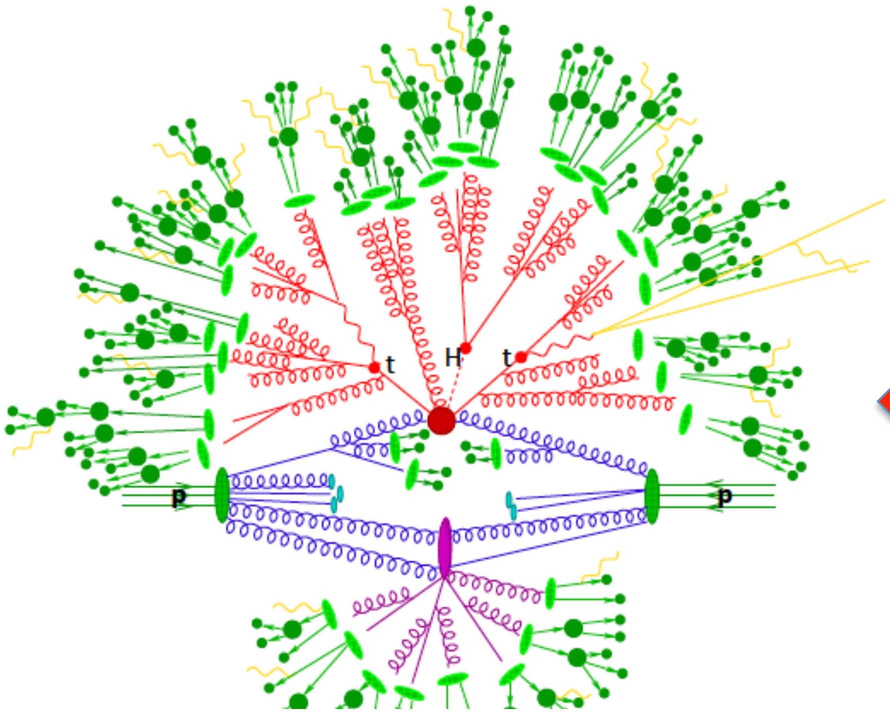
- use of the same parameters for the predictions of different observables
- Simultaneous Tunes to different observables
- Validation of models and tunes in direct comparison with different data sets

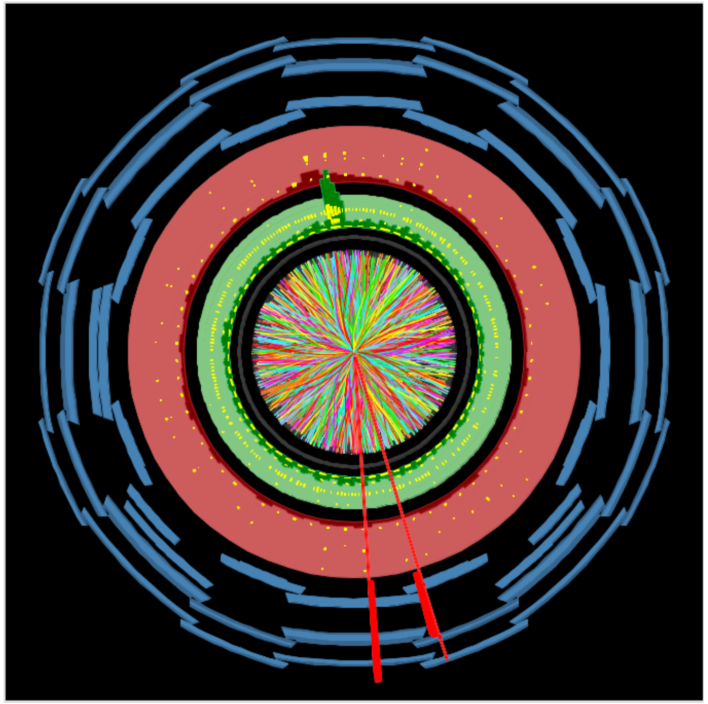
QCD models in MC



Up to ~30 tuneable parameters in MC codes

MC comparison to data





MC generator particles and jets

Particles and jets reconstructed from detector signals

Data-MC comparison

Details of MC-data comparisons (1)

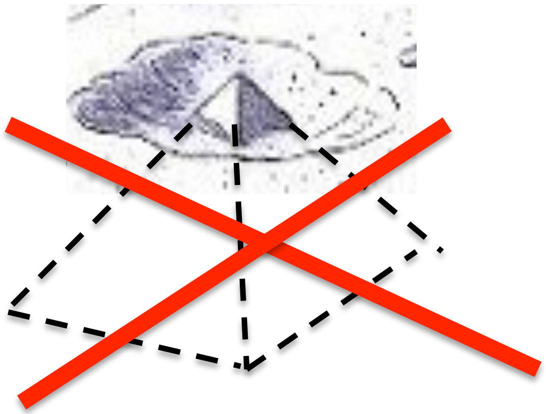
Fiducial volume

"This could be the discovery of the century. Depending, of course, on how far down it goes."

Details of data-mc comparisons (1)

"Visible" or Fiducial volume

Idea: limit model dependent correction by minimizing extrapolation in unmeasured regions



Details of data-mc comparisons (1)

“Visible” or Fiducial volume

Idea: limit model dependent correction by minimizing extrapolation in unmeasured regions

Kinematics:
Same kinematic phase space
MC particles as used in data analysis
e.g.
$|\eta| < 2.5$, $p_T > 25$ GeV, ….

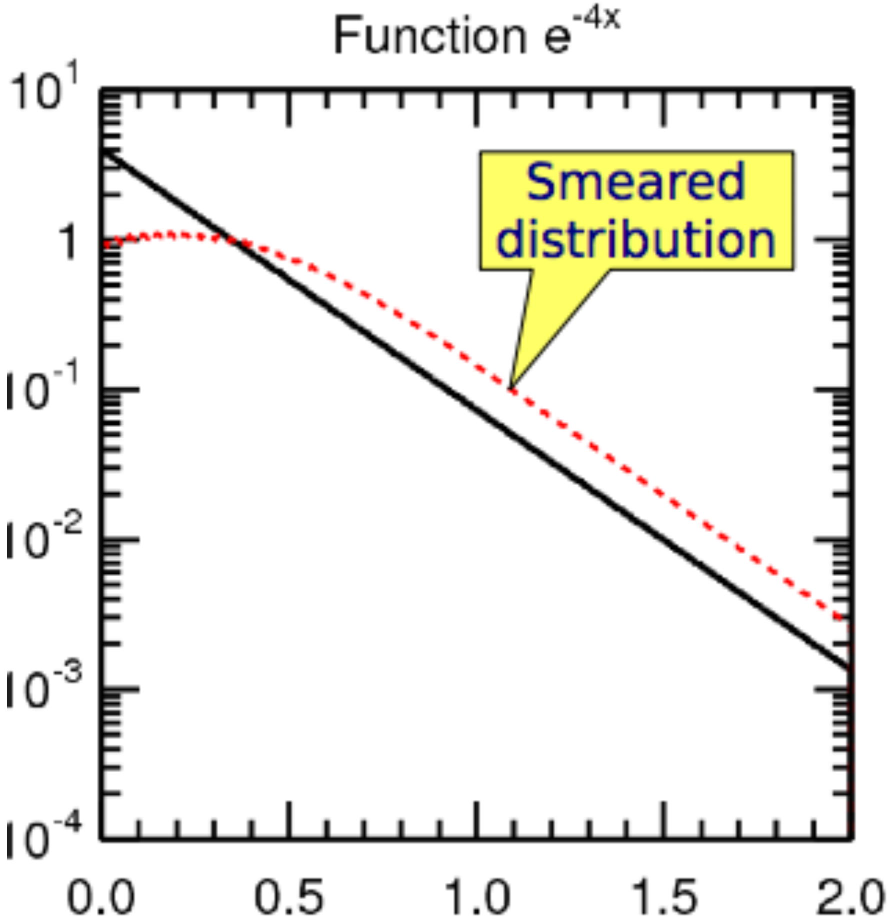
Particles/jets in MC corresponding to detectable particles/jets in data

- Use only stable MC particles in the final state
- **Jets** of stable particles reconstructed with anti-kt jet algorithm (R=0.4 ATLAS, R=0.6 CMS)
- **b-quark initiated jets** reconstructed as stable particle jets containing B-hadron with non-prompt electro-weak decays
- **Leptons “**dressed” with photons from QED radiation if they cannot be resolved due to limited detector resolution
- **ETmiss/Neutrinos** missing transverse energy is calculated as the 4-vector sum of neutrinos from W/Z--boson decays.

See standard defined by [LPCC working group]

Side remark:
Detector Resolution Effects

Example: Steeply falling distribution

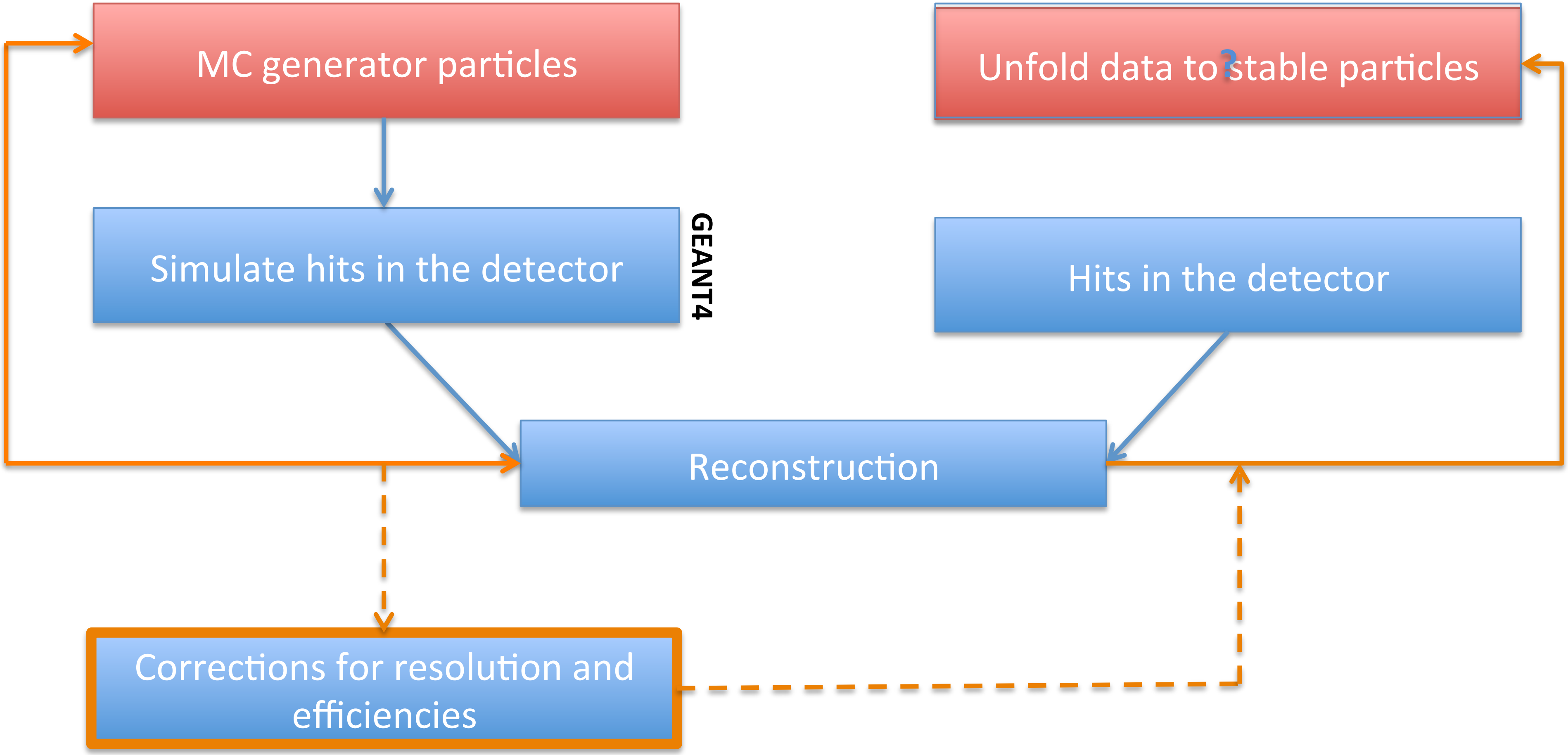


- Function e^{-4x}
- smeared by Gaussian with width of 0.3
- true and smeared (measured) distribution differ by large amount

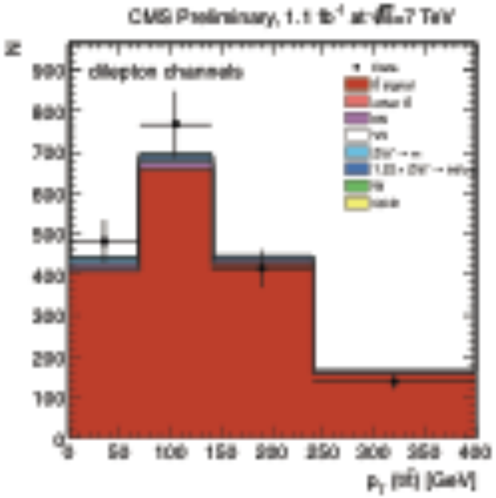
Measurement: unsmear ('unfold') measured distribution to retrieve true distribution

Details of data-mc comparisons

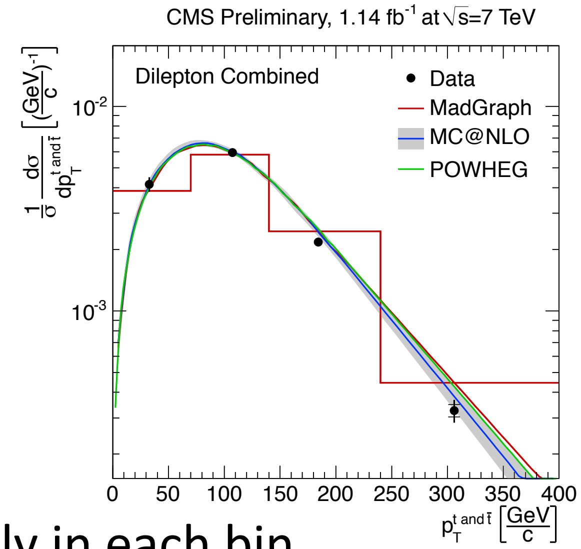
Unfolding



Simplest case: Bin-by-bin unfolding



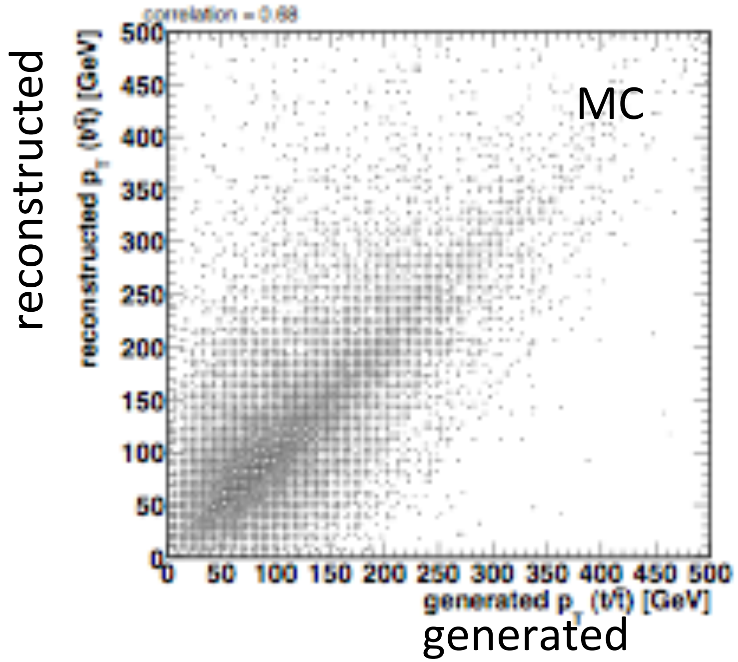
correct measured
Distribution back to
Parton level distribution
(unfolding)

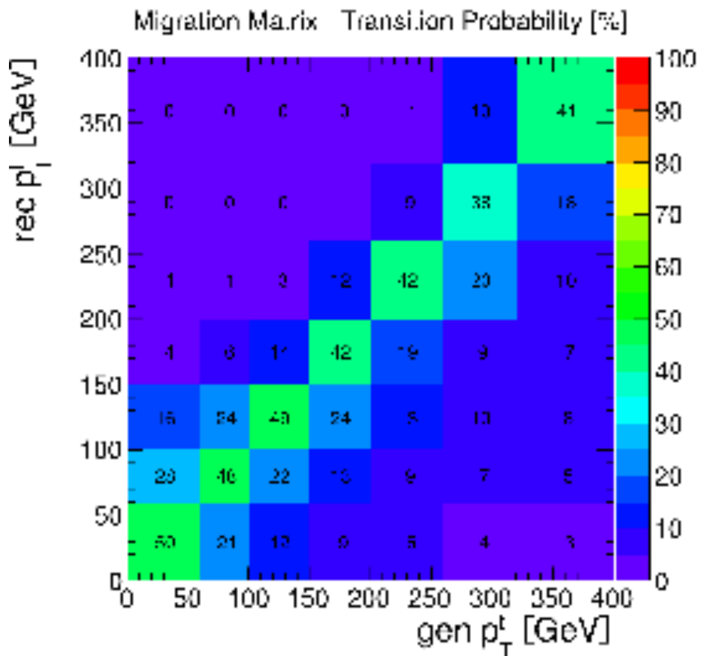


apply efficiency correction separately in each bin

- Features
  - simple, fast, robust, statistical errors are well defined sqrt(N), biases included in systematics
  - need good description of data, result does not include correlations

Full unfolding with response matrix





$$\vec{N}_{\text{Signal}} = A\vec{N}_{\text{true}}$$

$$\vec{N}_{\text{true}} = A^{-1}\vec{N}_{\text{Signal}}$$

$$p^i = \frac{N^i_{rec\&gen}}{N^i_{rec}}$$

$$s^i = \frac{N^i_{rec\&gen}}{N^i_{gen}}$$

sensitive to migration

p^i: into bin i

s^i: out of bin i

Choose bins such that purity and stability are larger than 40-50%

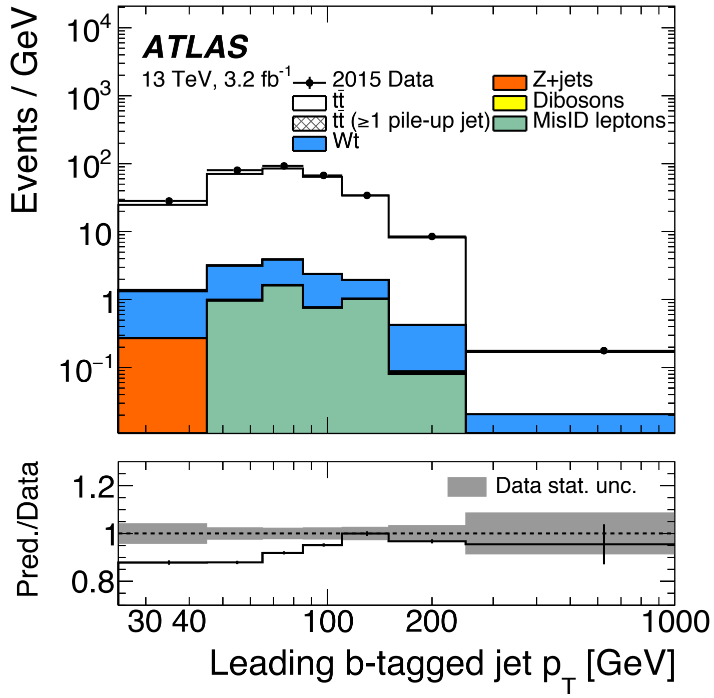
Full unfolding using full response matrix

- yields full covariance matrix
- slow and complex

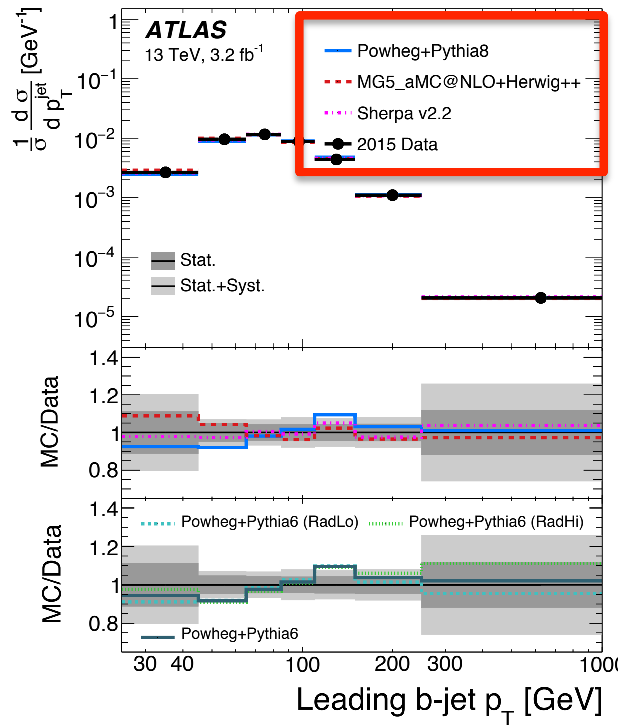
Result of full unfolding

Example: highest p_T b-jet in top pair production

Reconstruction Level

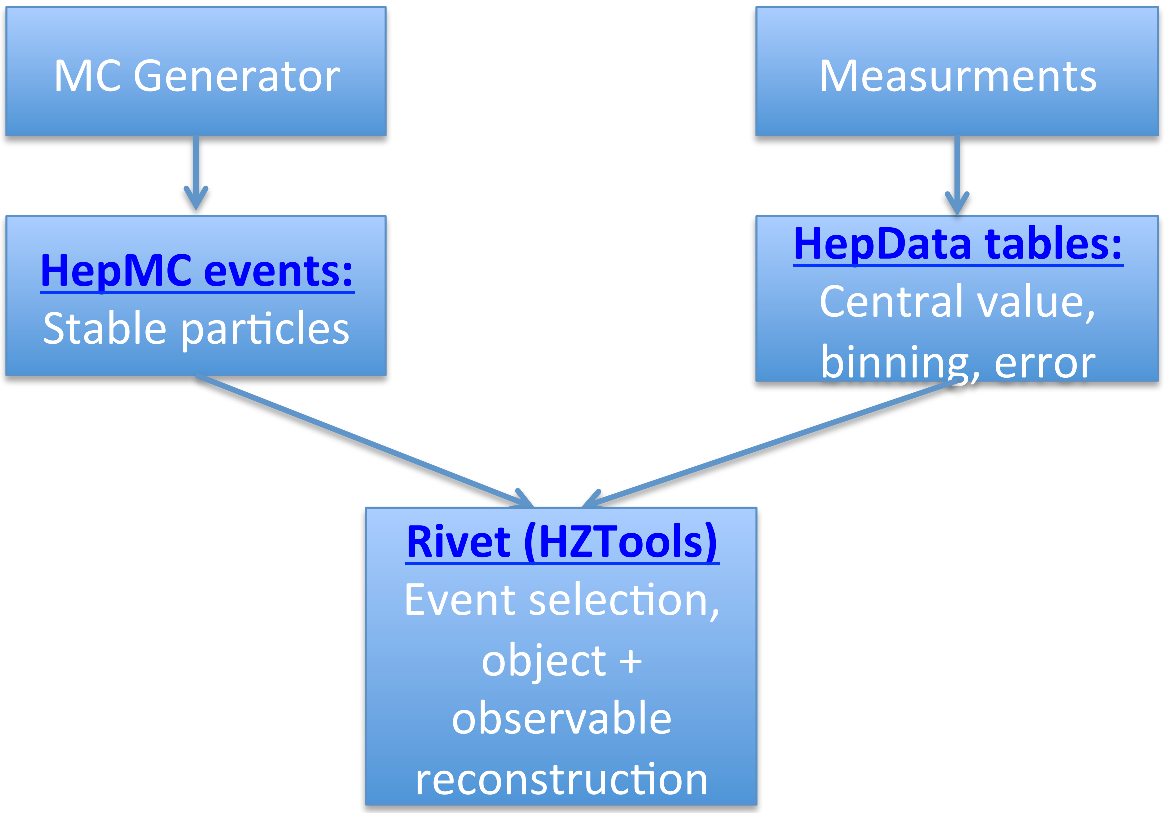


Particle Level



MC-Data Comparisons

Data-MC comparisons
Tools



MC Tuning Methods

- Assumption: each parameter controls only a relatively small & exclusive detail of the event generation
  - Allows tuning of small amount of parameters for a particular component to suitable observables
  - However, observables are usually also weakly dependent on other parameters & components
  - Iterative tuning
- Typical tuning sequence:
  1. Fragmentation and parts of parton shower tuned to LEP data
  2. Soft QCD models tuned to hadron collider data
- Probe scaling of models by tuning / comparing to different cms energies (Tevatron, LHC 900 GeV, 7 TeV, 8 TeV, 13 TeV)

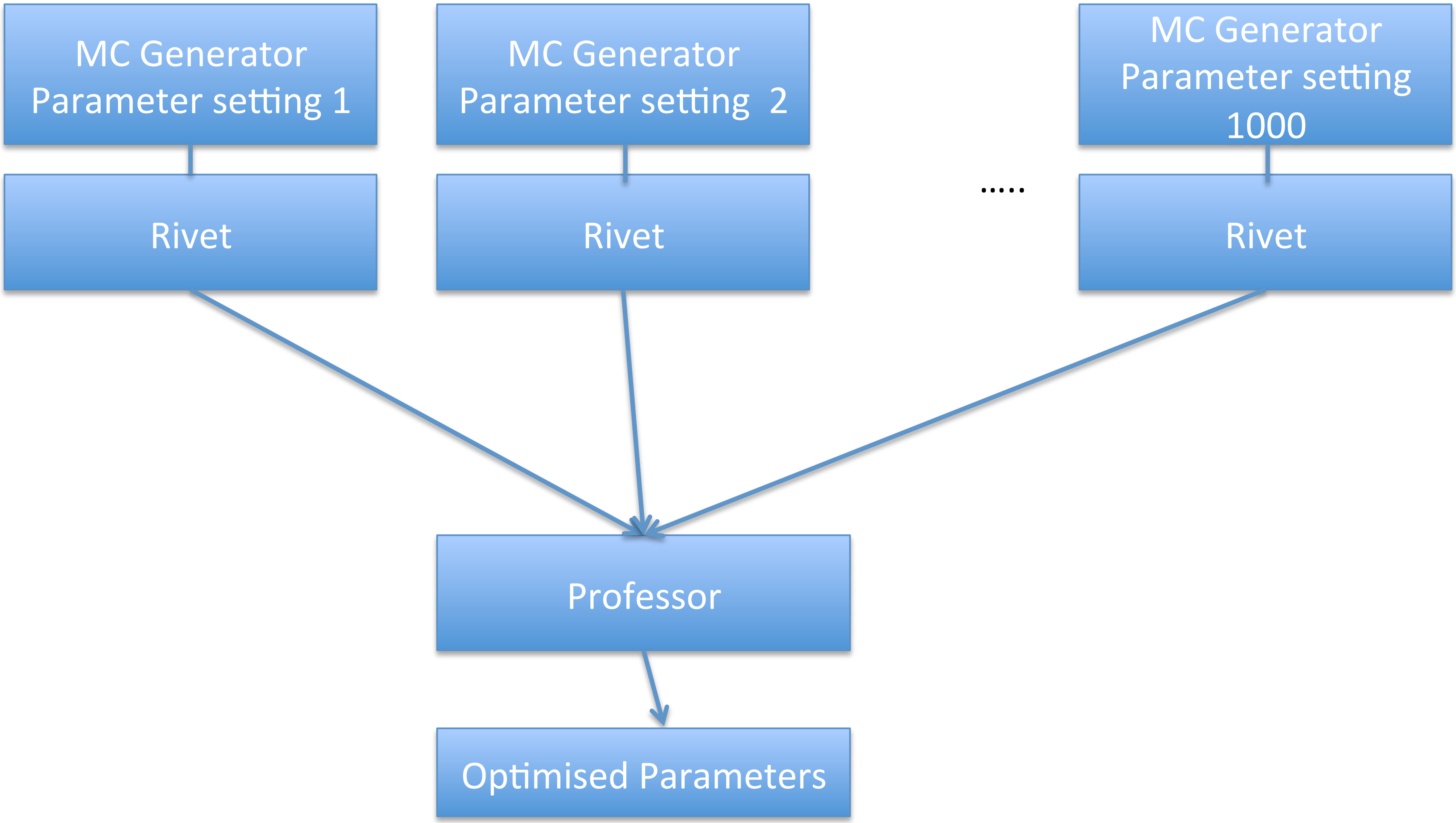
Tuning methods (1)
Manual tunes

- Generate predictions for a parameter set within the validity range of the model & optimise according to human judgement
- Strength: comprehensible & stable results
- Limitations: correlated and many parameters -> very time consuming
- Examples: Pythia6 and Pythia8 author (Skands, Sjoestrand) tunes (Perugia Tunes, Monash Tunes, C4, C4x…), tune A, Z1, Z2, (Rick Field)

Tuning method (2)
Analytical approximations

- Approximate the parameter dependence of the physical observable on the model parameters by an analytical function, typically a 2nd or 3rd order polynomial
- Optimise tuning of a large number of parameters simultaneously
- Originally method developed at LEP, reimplemented in Professor Tool
- Personal judgement enters via weights of observables
- Examples: ATLAS tunes (pythia AMBT1, AZ, AUET, fHerwig), CUET tunes, recent Herwig++ and Sherpa tunes

Tuning chain



Uncertainties on models & optimised parameters

- Tuning to different but redundant observables or different ranges of observable spectra (AZ tunes)
- Allow limited deviations from the measurements (see Perugia tunes)
- Perform "eigentunes" of the analytical approximation: calculate chi2 variations of the diagonalised covariance matrix used in the minimisation (see ATLAS tunes)

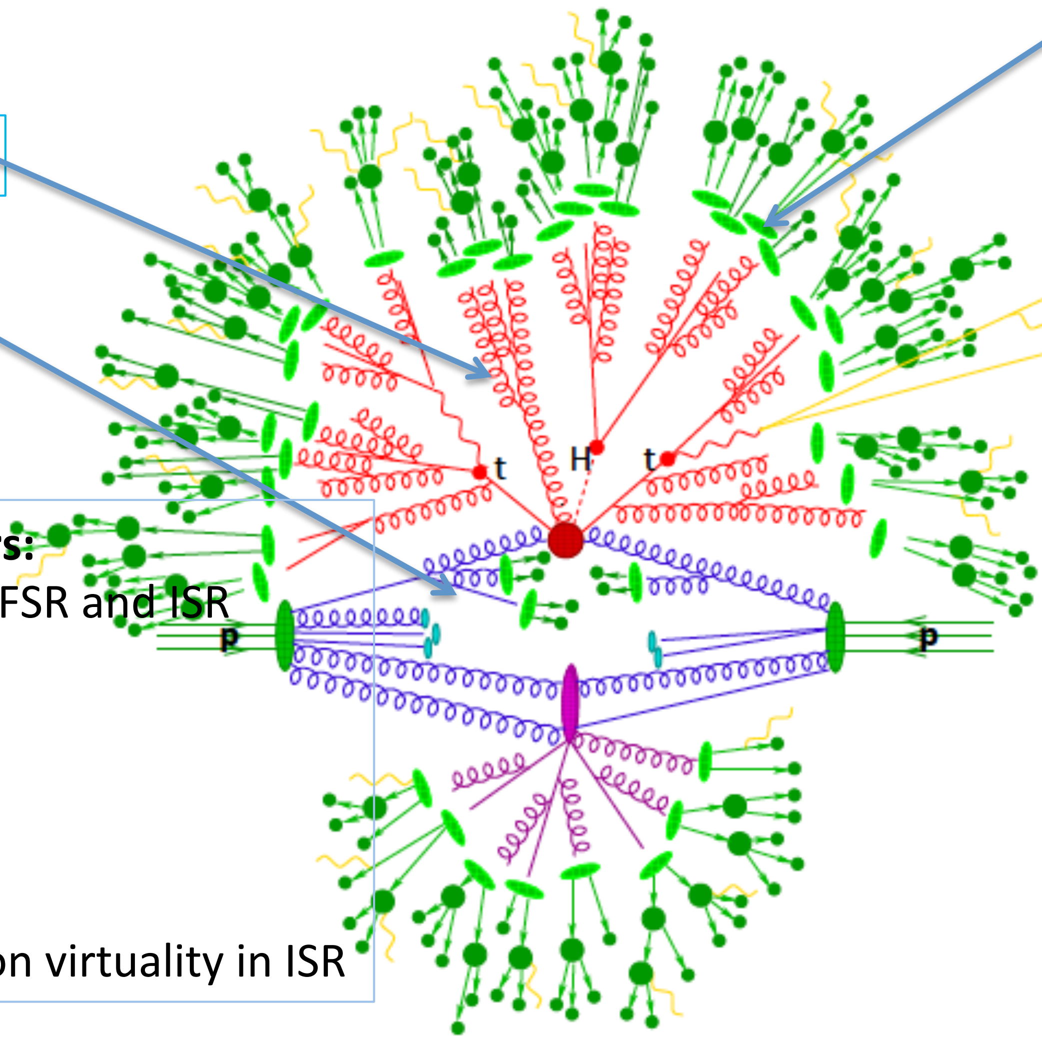
Tuning parton shower and fragmentation

QCD FS radiation

IS QCD radiation

Hadronisation of
Final state partons

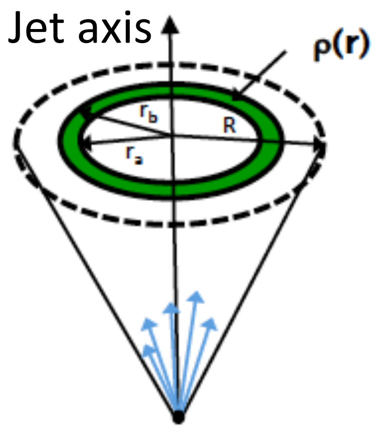
Lund string model or
Cluster fragmentation



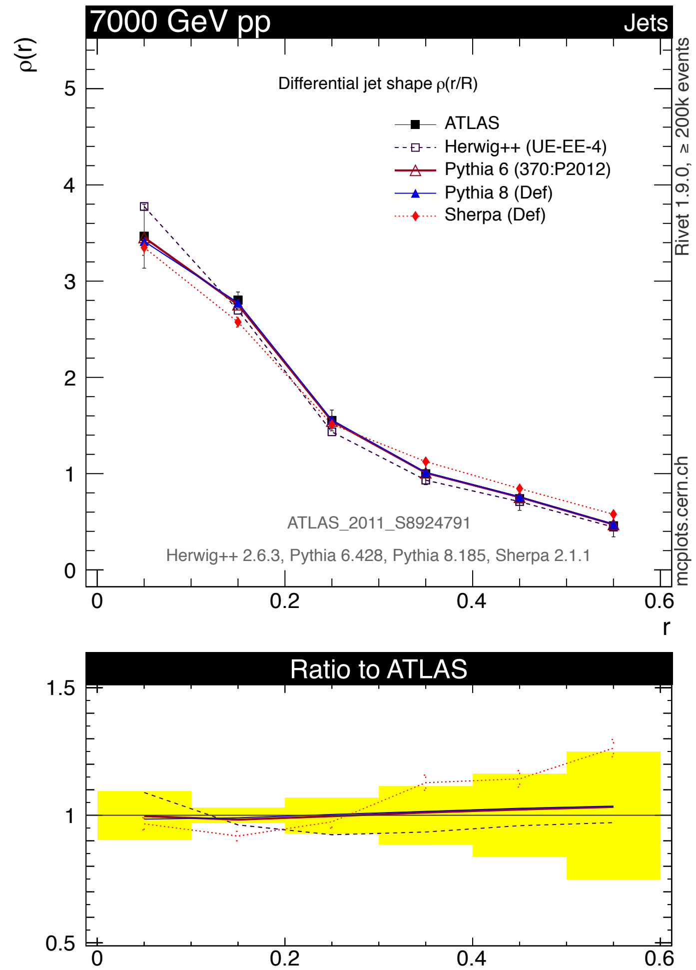
Tuned to LEP data:
- particle multiplicity
- Event shape variables
- Momentum spectra

Shower parameters:
Low Q_0 cut-off for FSR and ISR
α_s (λ_{QCD}) for FSR
Mean intrinsic k_T
PYTHIA:
α_s for ISR
α_s for FSR off ISR
Max. allowed parton virtuality in ISR

Observables sensitive to Final State Radiation and Fragmentation: Jet shapes



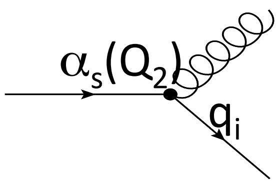
$$\rho(r) = \frac{1}{\delta r} \cdot \frac{1}{N_{jets}} \cdot \sum_{jets} \frac{p_T(r_a, r_b)}{p_T(0, R)}$$



In ,many bins of jet pT

MC parameter:

α_S in FSR



+ b-jet shapes, jet shapes from Tevatron

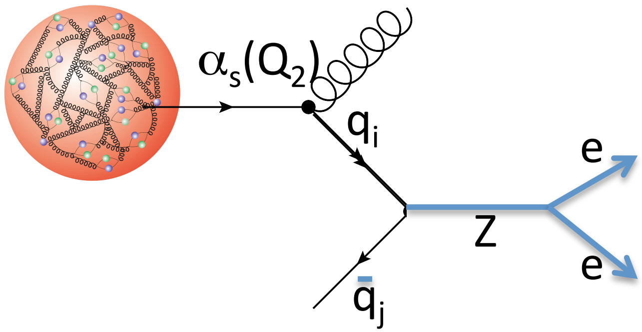
Initial State Radiation Observables: Drell Yan

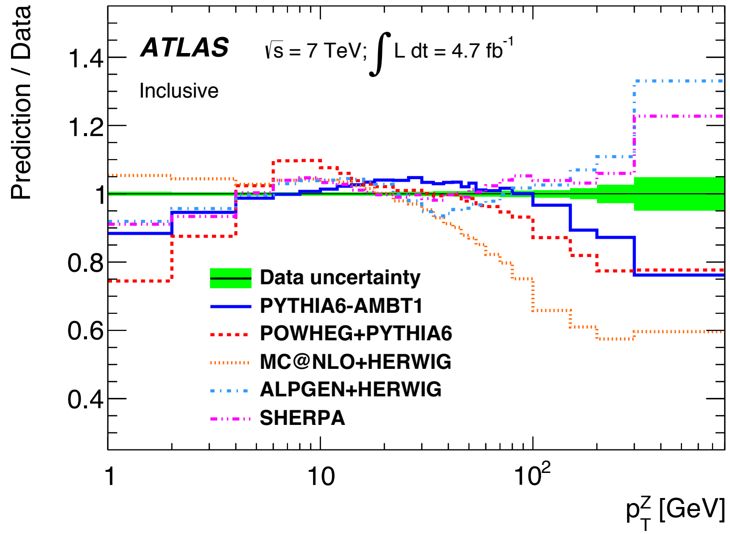
Observables: p^Z_T and phi*

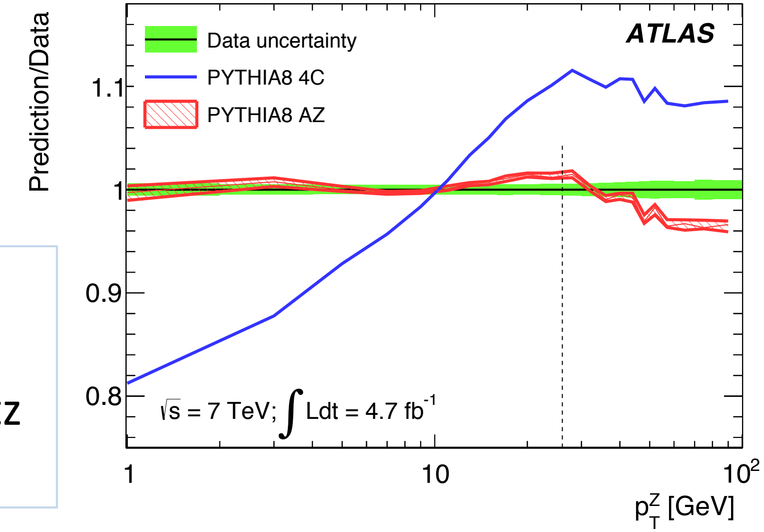
$$\phi^*_\eta \equiv \tan(\phi_{acop}/2) \cdot \sin(\theta^*_\eta)$$

Intrinsc k_T:
k_T of partons inside incoming protons
Fermi motion ~200 MeV
"sum of unresovled effect below shower cut-off"

ISR cut-off: Q_0
α_S(ISR)



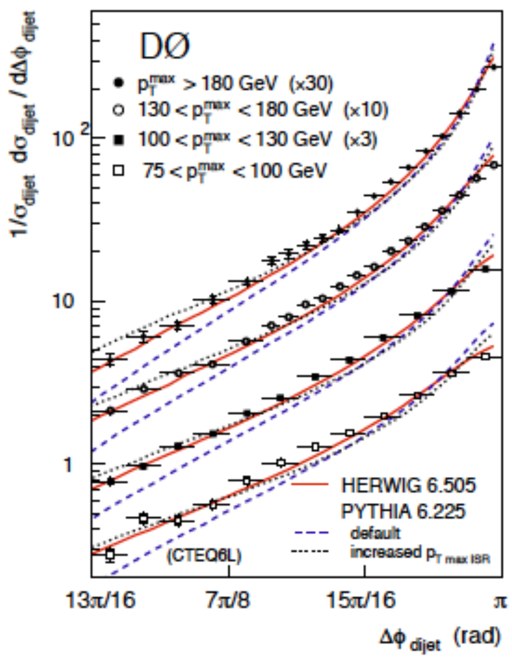


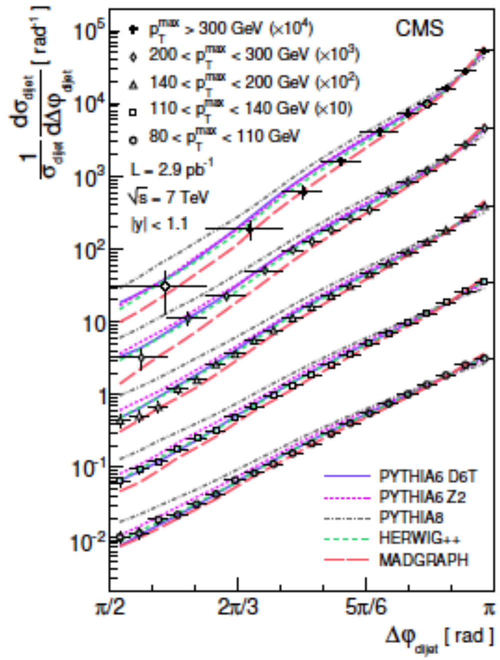


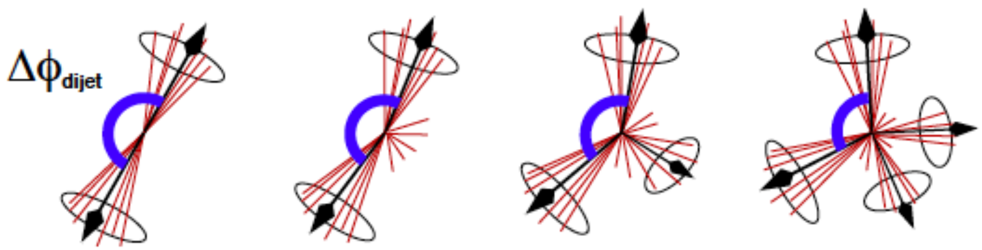
Pythia has separate α_S for ISR and FSR to effectively incorporate various soft effects
Herwig has only one α_S for parton shower to keep Lorentz Invariance

Parton Shower Tuning in dijet decorrelation

Probe hard and soft emission without explicit separation

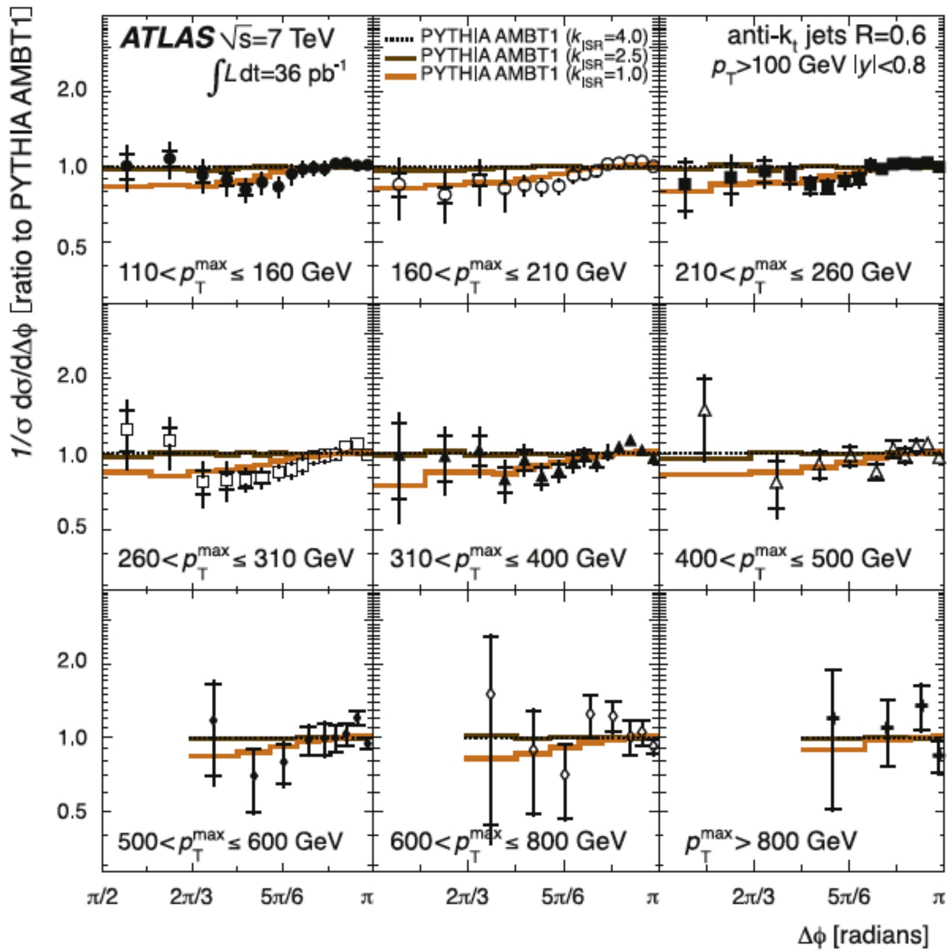




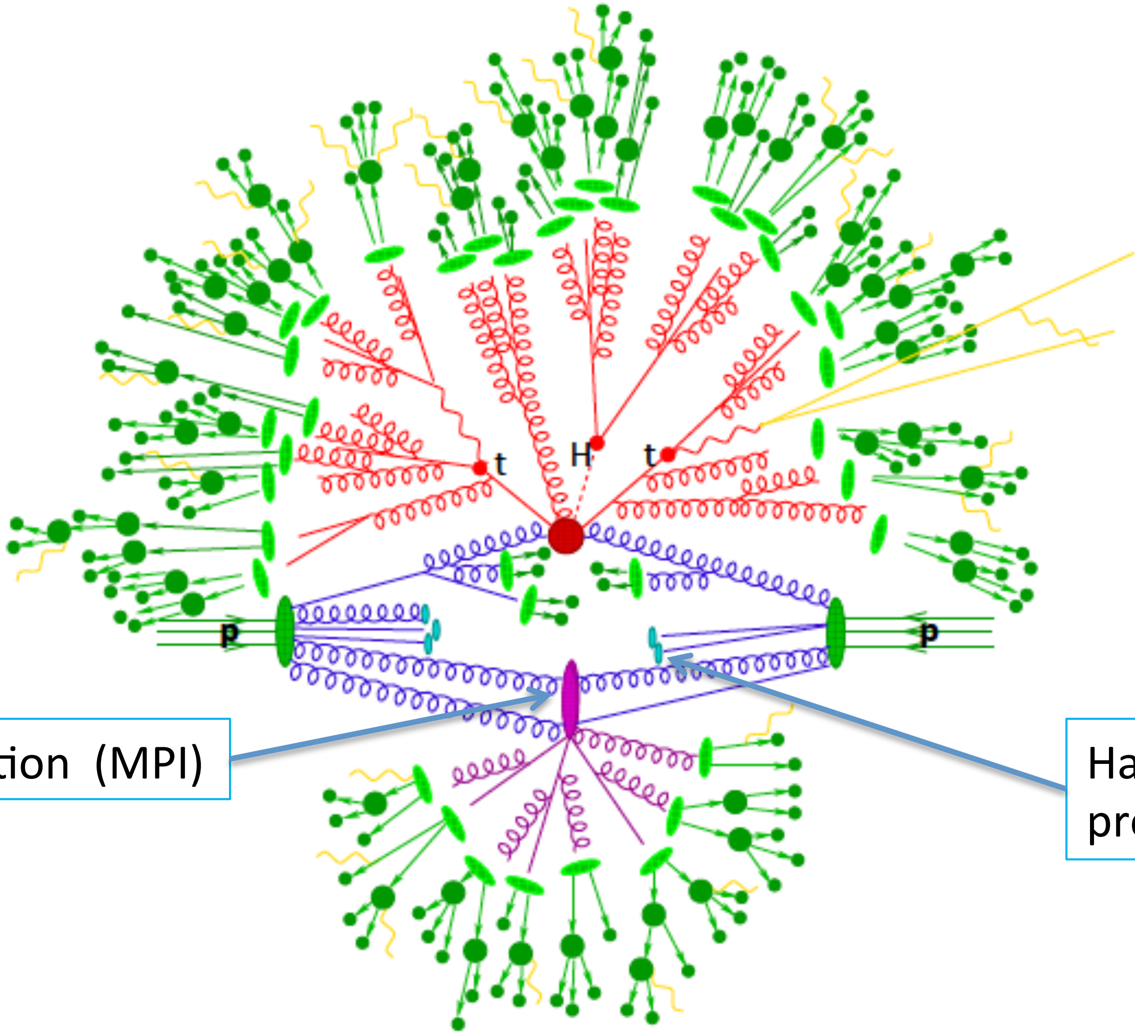


Sensitive to max. allowed parton virtuality in ISR

Pythia6 Shower Tuning in dijet decorrelation



MPI and Colour Reconnection

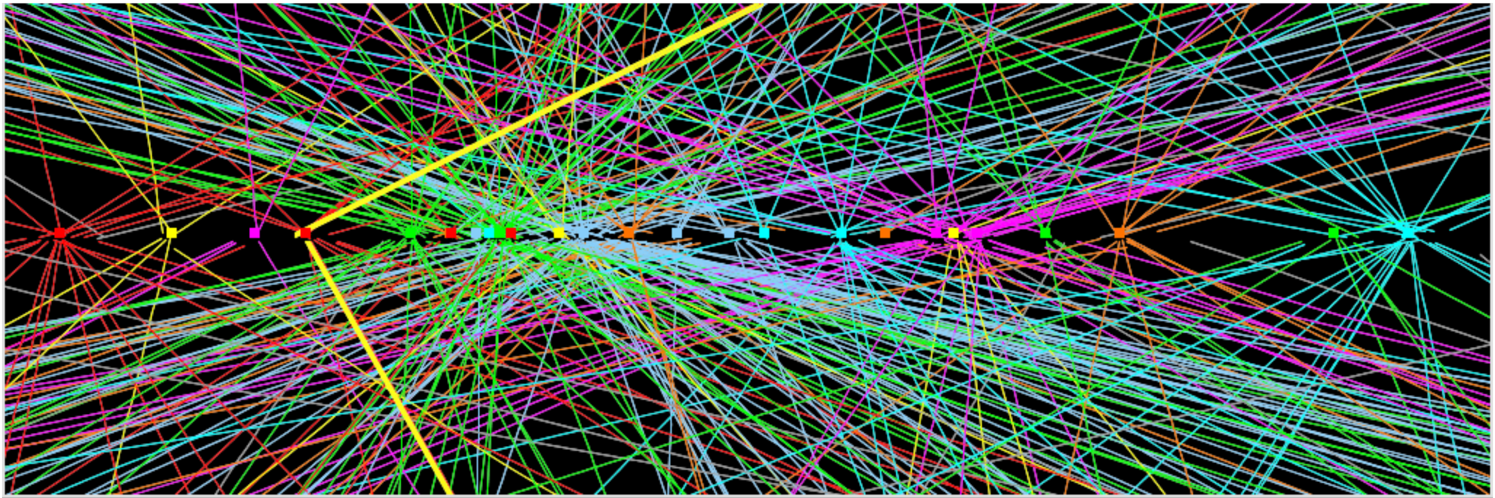


Secondary interaction (MPI)

Hadronisation of proton remnant

Reminder: Minimum bias abundantly

Pile-up at LHC

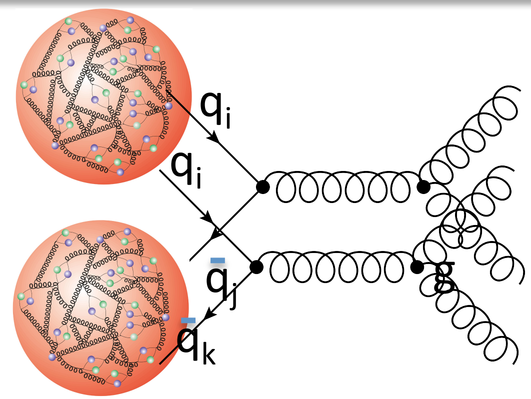


2012 data (8 TeV): <mu> ~ 21

Run 2 (13-14 TeV): <mu> ~ 40

High Lumi LHC: <mu> ~ 400

Multi-parton interactions



- Secondary interaction between remnant partons
- Modeled by perturbative parton-parton scattering framework

  -> rising towards low p_T

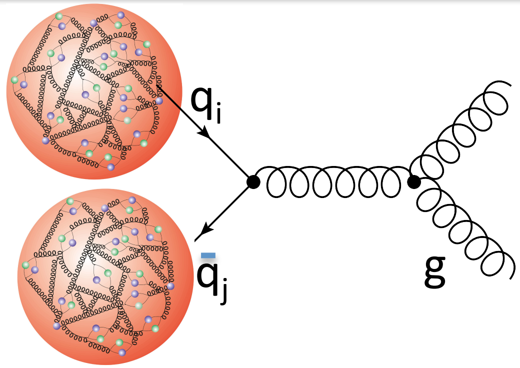
  -> dominated by t-channel gluon exchange

  -> parton shower and hadronise
- Hard MPI observed gamma+2jet (Tevatron), W+di-jet and 4 jet production (LHC)
- Soft MPI: major source of soft particle production in min.bias events and underlying event in hard scatter processes

Further reading: arXiv:1706.02166v1

MPI model & parameters

$$\sigma_{hard}(p_{T,min}) = \int_{p^2_{T,min}}^{s/4} \frac{d\sigma}{dp^2_T} dp^2_T.$$



- Exceed total cross section at 1-2 GeV due to high parton densities
  - Limit rise of partonic cross section via
    N(parton-parton) = sigma(hard)/sigma(non-diff) -> matter overlap
- Divergent for pT->0 : introduce cut-off pTmin

$$p_{T,min}(\sqrt{s}) = p_{T,min,0} \cdot (\frac{\sqrt{s}}{E_0})^b$$

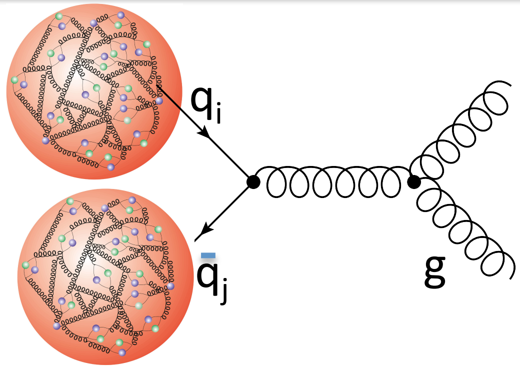
MPI parameters dependent on Parton Densities (PDF)!

Tuneable paramters

Further reading: arXiv:1706.02166v1

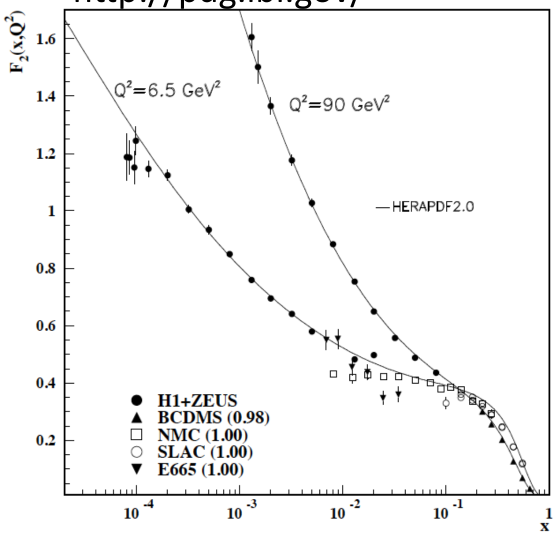
MPI model & parameters

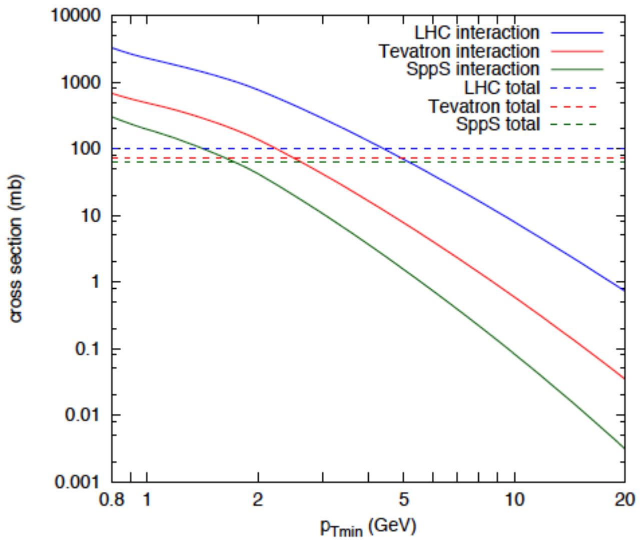
$$\sigma_{hard}(p_{T,min}) = \int_{p^2_{T,min}}^{s/4} \frac{d\sigma}{dp_T^2} dp_T^2.$$



- Exceed total cross section at 1-2 GeV due to high parton densities

http://pdg.lbl.gov/





MPI parameters dependent on Parton Densities (PDF)!

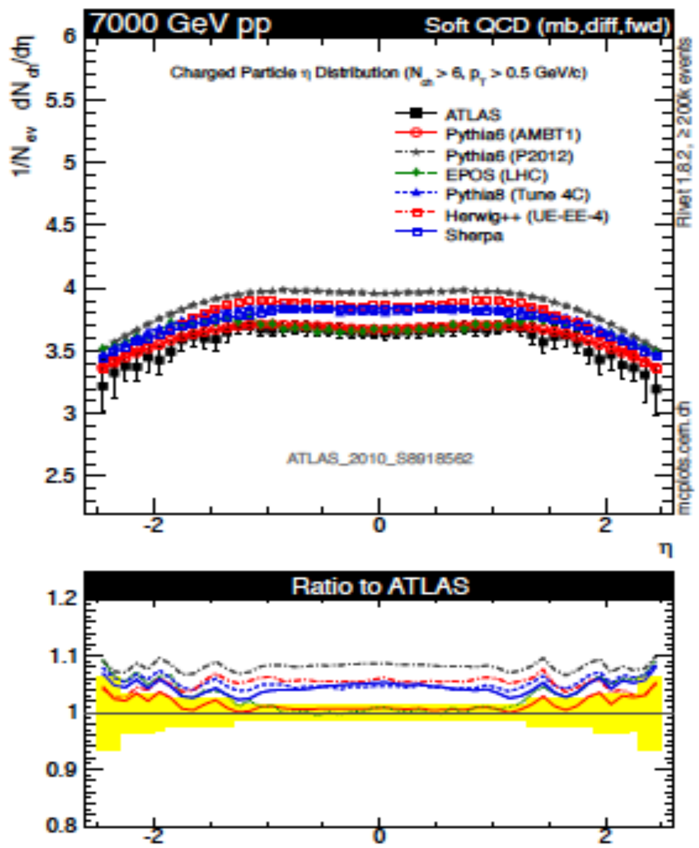
Observables and model parameters for MPI

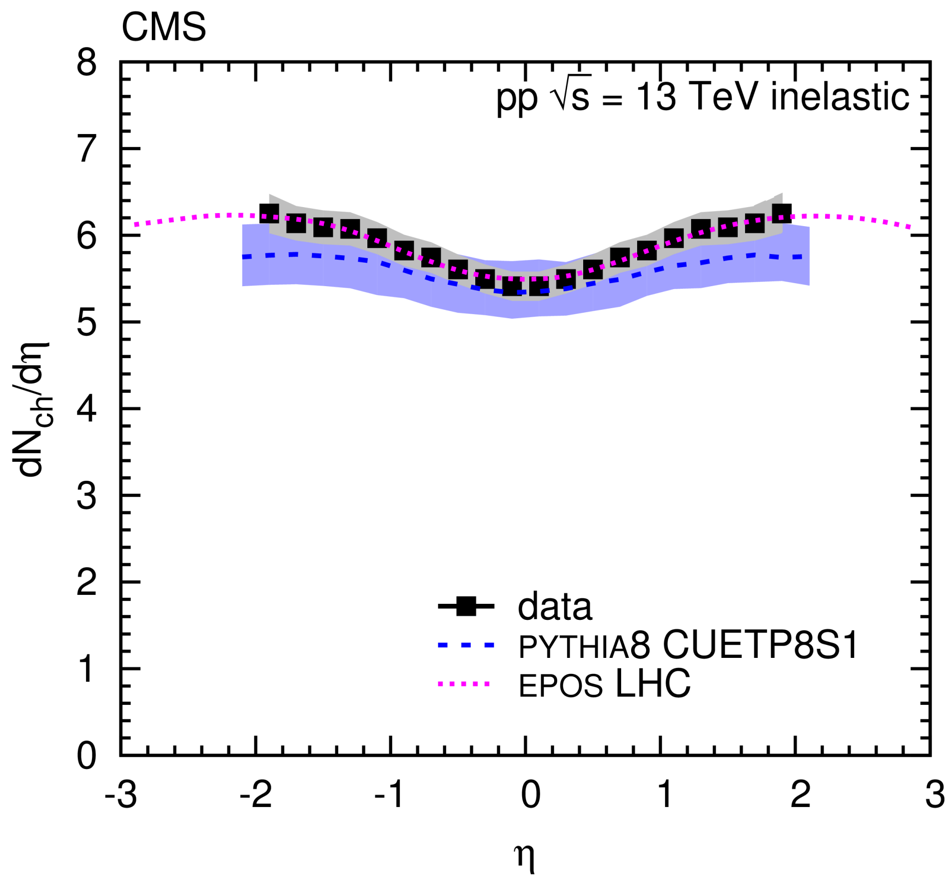
Mean nr of charged particles (Ncharged) : ptmin,0

Charged particles at different sqrt(s) measured at LHC, Tevatron, SPS

Probability distribution of charged particle multiplicity: matter distribution

Minimum Bias Measurements (1) charged particle distributions

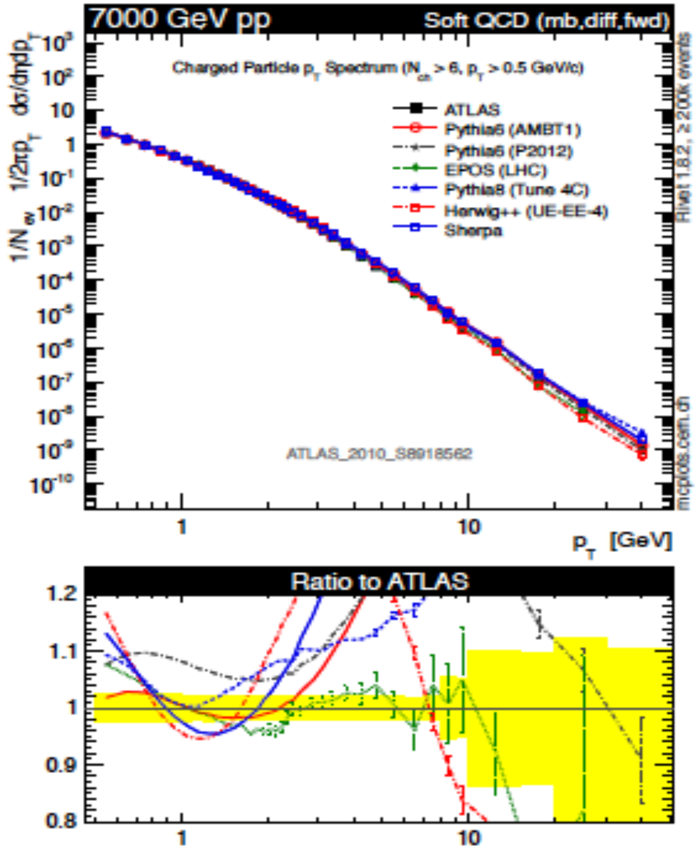


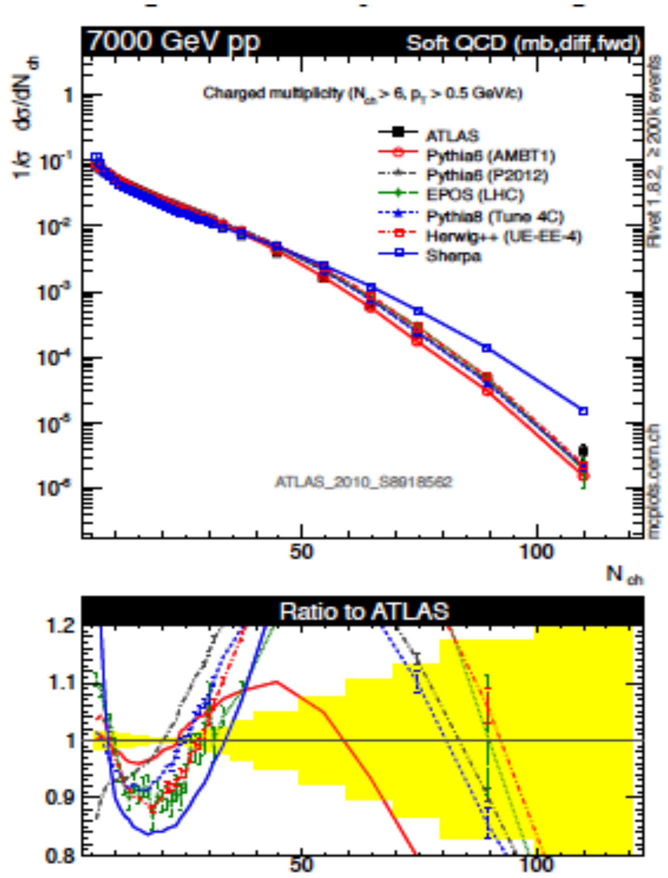


Check theory extrapolation and re-tune if needed for each new center of mass energy!

EPOS LHC: tuned to 7 TeV data

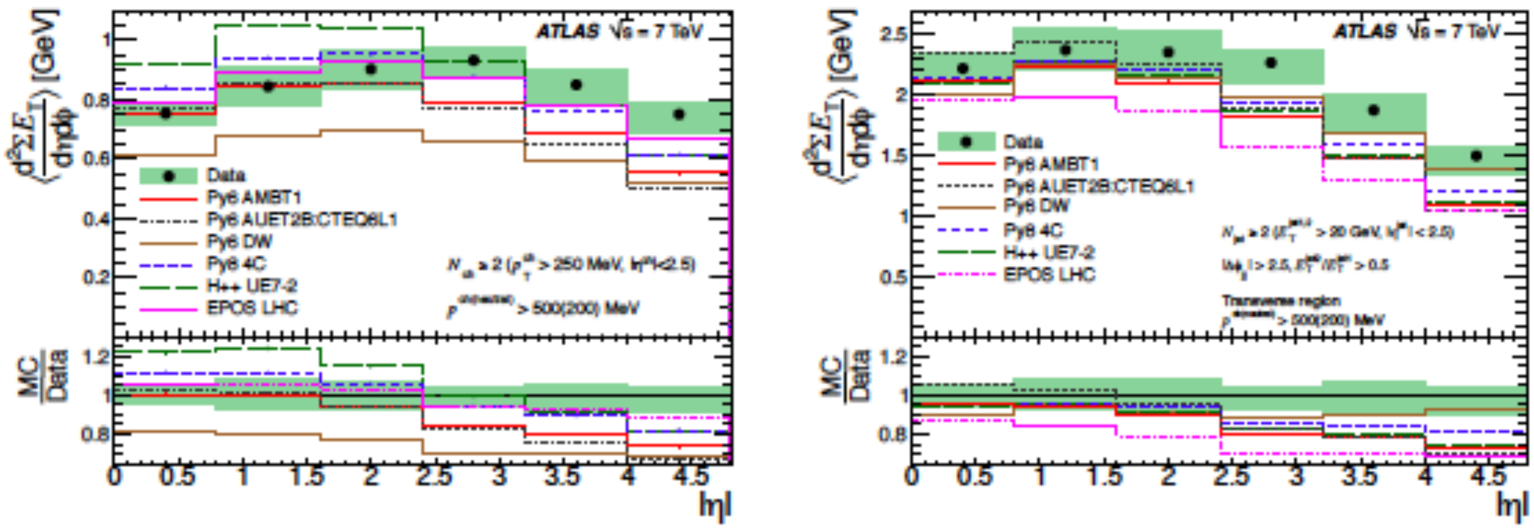
Minimum Bias Measurements (2) momentum spectra





Difficult to get momentum spectra, particle multiplicity and hadron composition right!

Minimum bias observables (3)
Neutral particles: energy flow



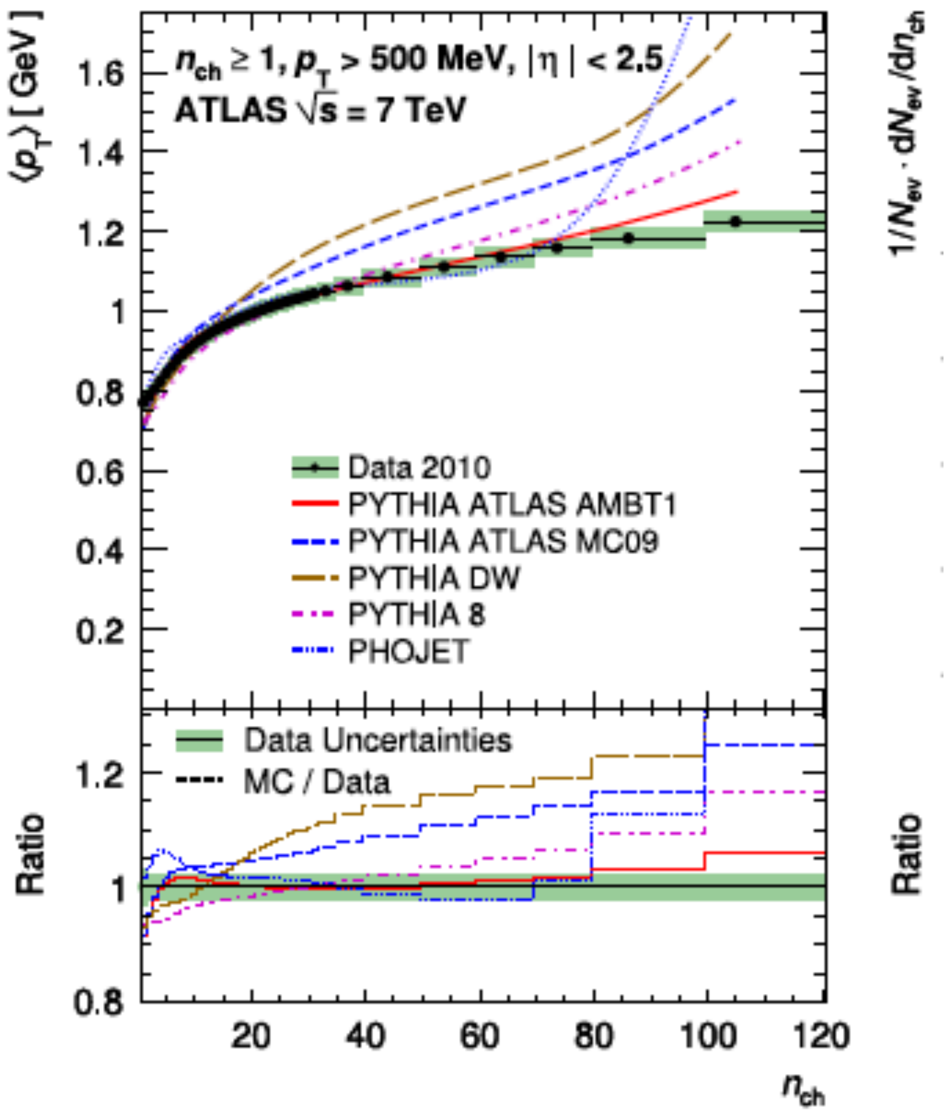
Hard to get right!

Would be nice to have for Etmiss and Cosmic rays……

Color reconnection

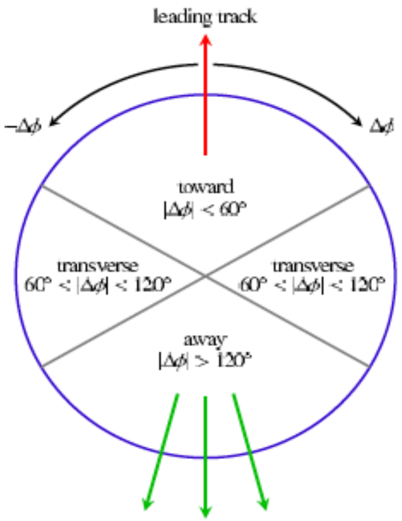
- Rearrangement of the final state parton connections due to the colour structure of the scattering
- Includes modeling of MPI scatters and colour flow in beam-beam remnant
- Various models exist, e.g. reorder hadrons to minimise string length or cluster mass
- Modifies the relation between <pT> and number of charged particles in hadron collisions
- May also affect top mass (one of the dominant uncertainties!)

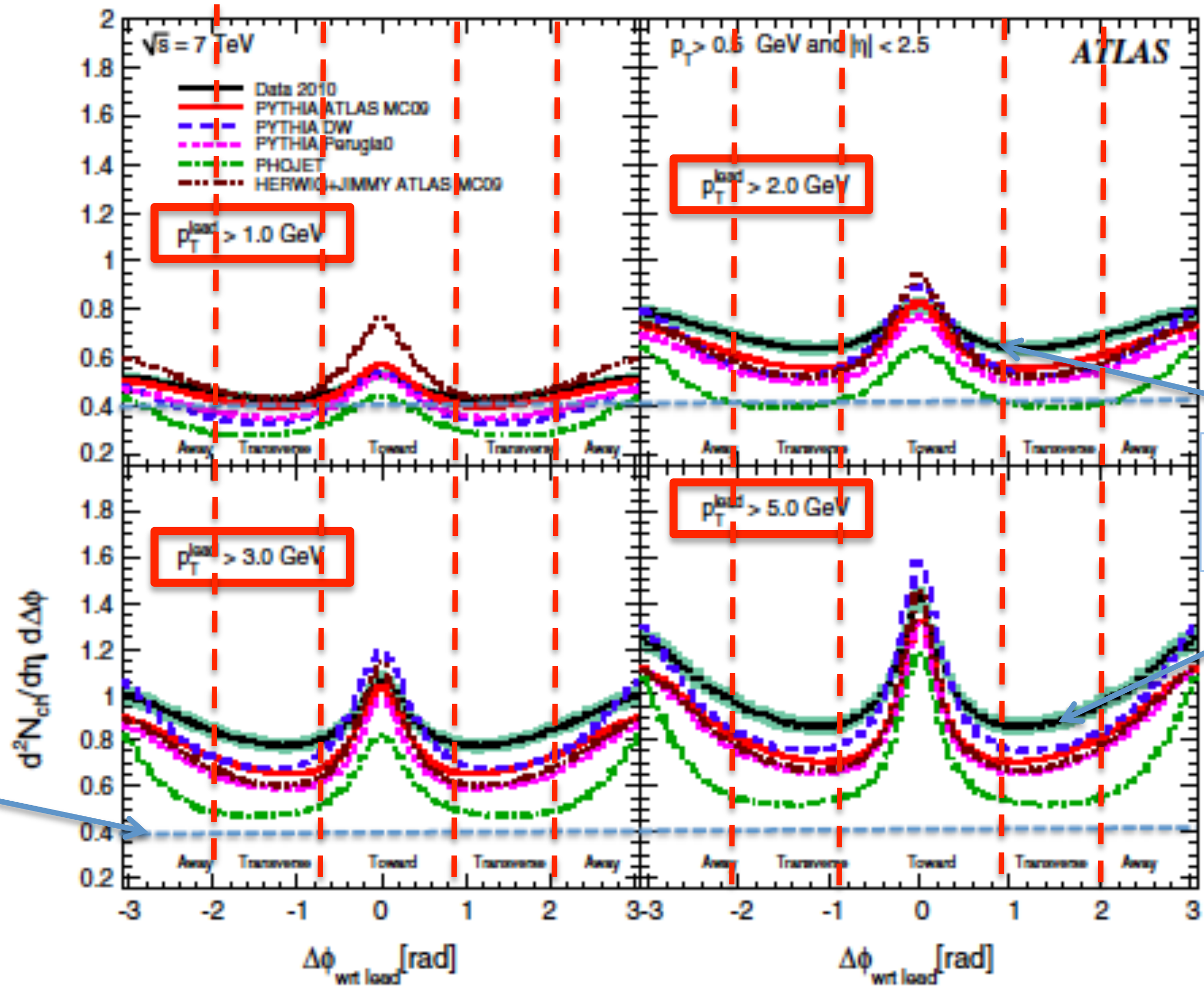
Color reconnection
Observables and model parameters



Parameter examples:
Pythia6: string length
Herwig6: Cluster size

Pedestal effect





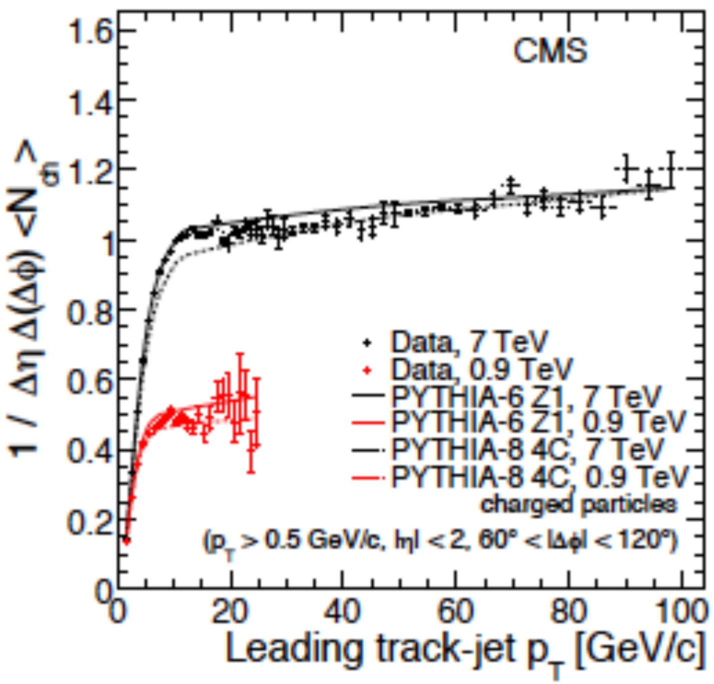
Pedestal below jet

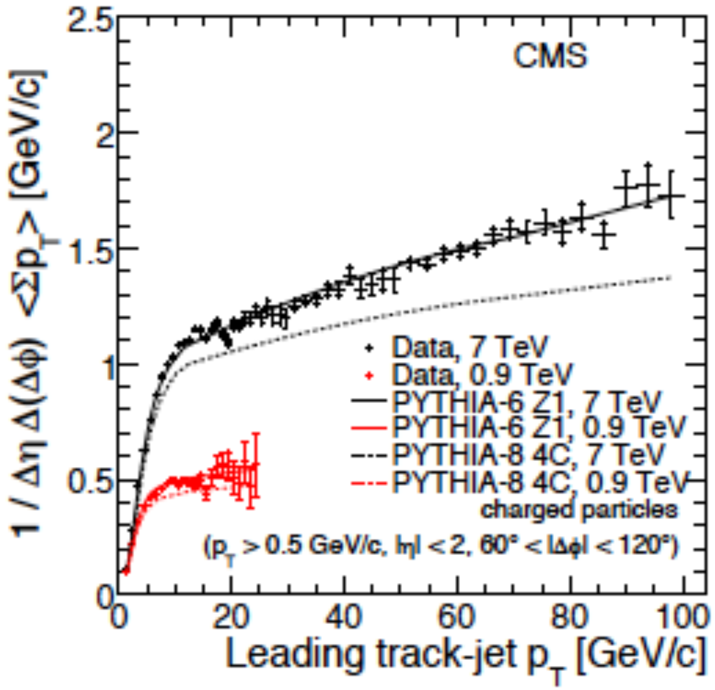
Minimum bias

Charged particle production with respect to the leading track

Underlying event observables

Measure charged particle density and energy density

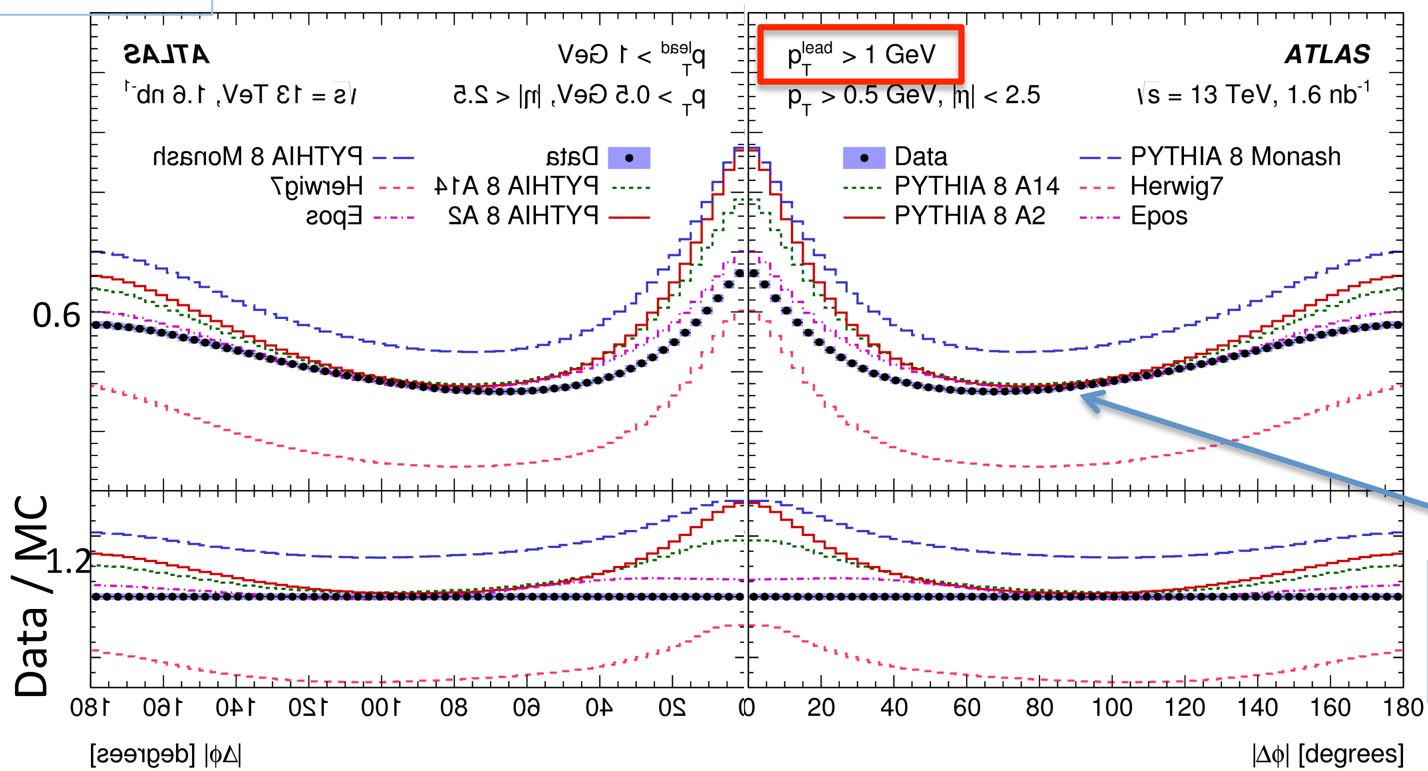




Good description achievable with LHC data at different CMS energies
Tension with Tevatron data

Pedestal effect @ 13 TeV

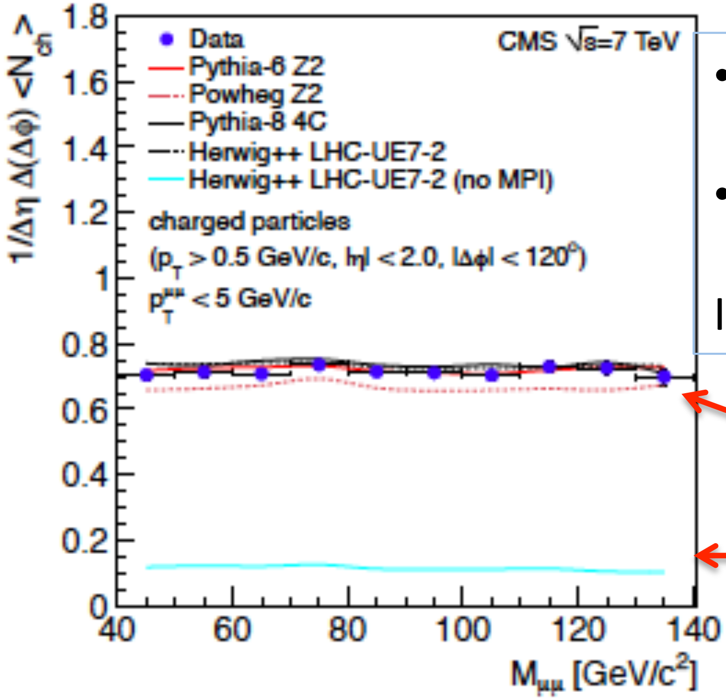
Minimum bias



Pedestal below jet

Modern generators and tunes still have difficulties to describe this completely

Disentangle ISR and MPI? Underlying Event in DY



- Measure particle production by removing the 2 muons
- No QCD radiation from the (LO) hard process

Ideal case to study MPI!

with MPI

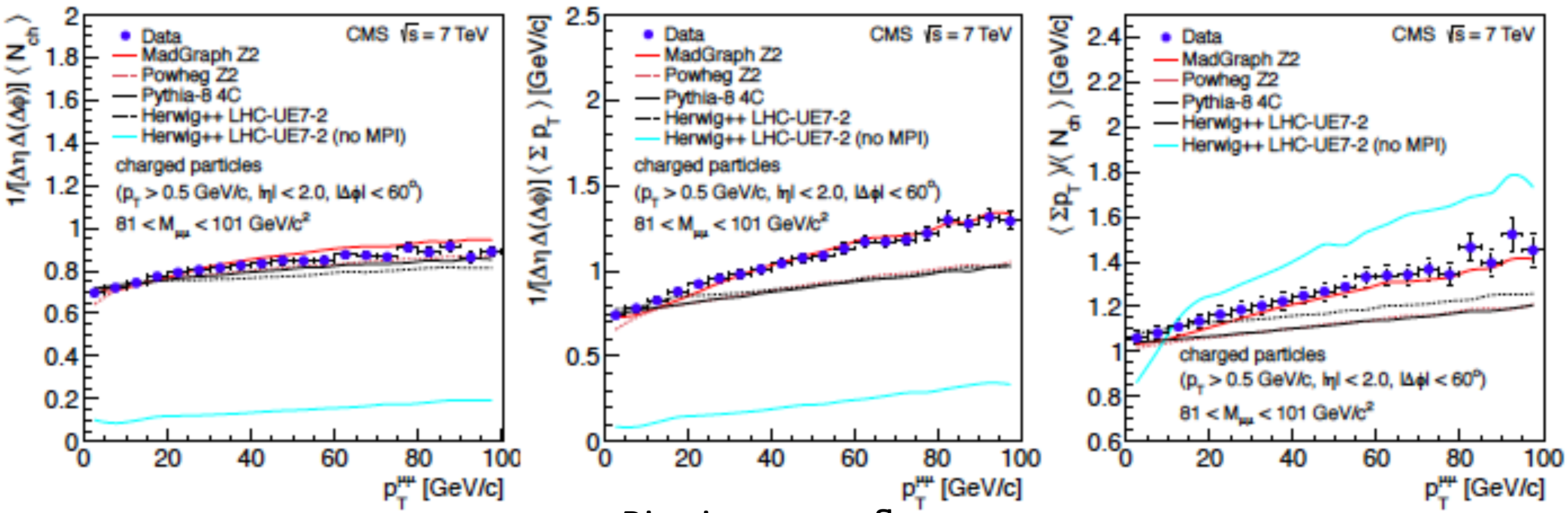
No MPI*

Large amount of particles produced by MPI

*Note: MPI interleaved with Parton Shower in PYTHIA -> kinematics change if MPI is switched off

Disentangle ISR and MPI?
UE in DY

particle density | energy density | ratio of energy and particle densities



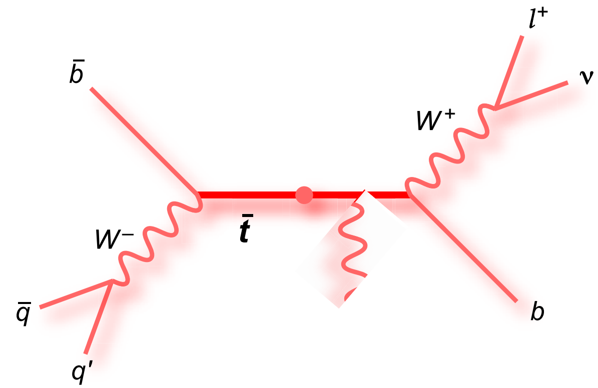
~stable particle production

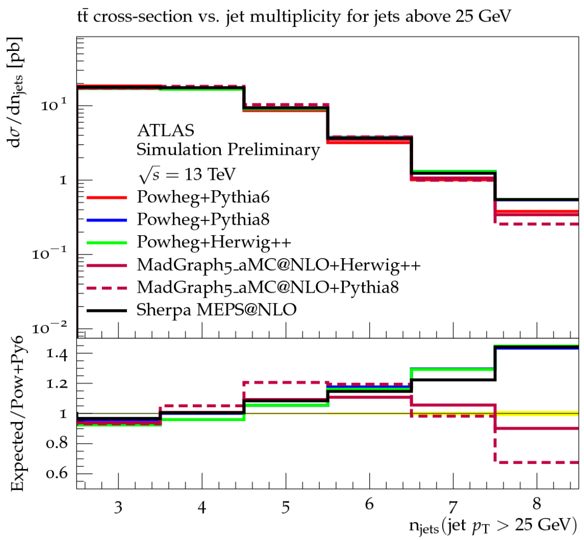
Rise in energy flow

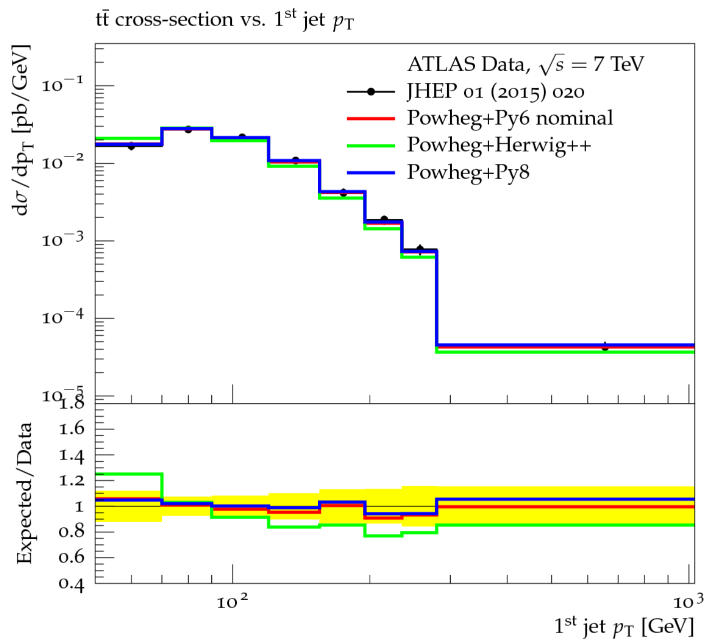
Significant contribution from ISR to UE

Description of final states at high scales: top pair production

Measure b jets plus decay products of W (single-lepton, di-lepton) and additional QCD radiation



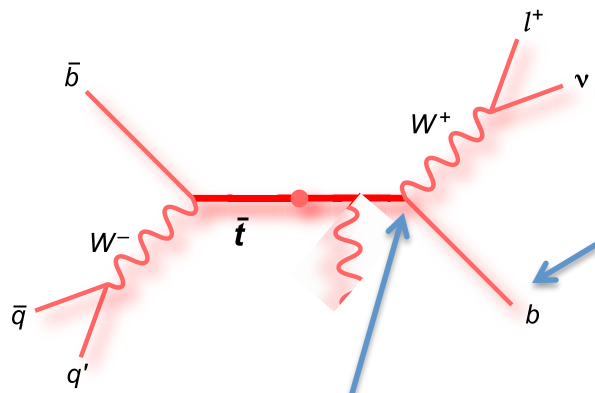




Tune

Simple picture: MC description of top decay products

Experimental signature b jets plus decay products of W
(single-lepton, di-lepton, all-hadronic)

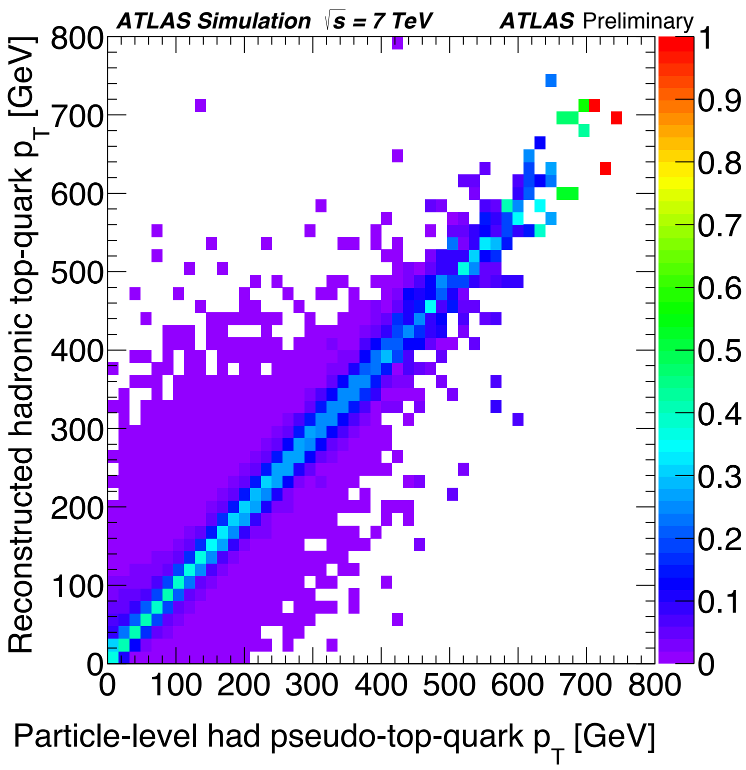


How to get it from stable particles in final state?

Top decays before hadronisation*

*Remember: fiducial measurements use stable final state particles!
Intermediate particles (top) are not observable and there is no common agreement what to Put into the MC event record. Usually, the analyses use the top quark that enters the decay vertex to W and b for parton level results.

Pseudo-top method

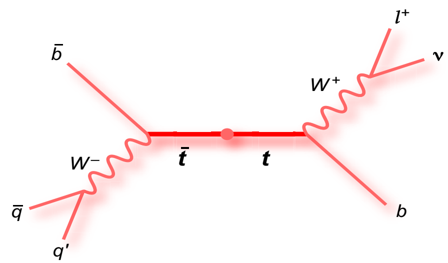


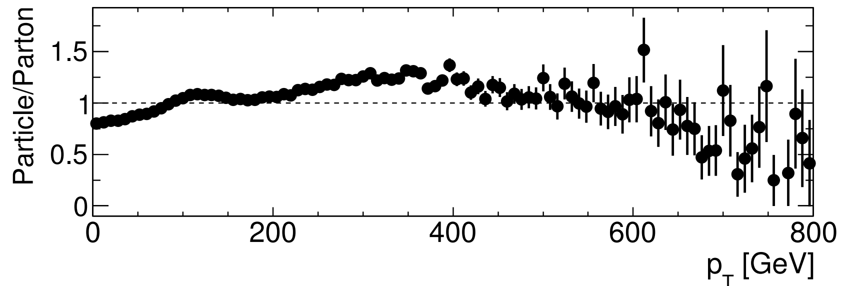
Assumed top decay products:
2 highest p_t b-jets, lepton, 2 highest p_t jets

Hadronic top:
b-jet,

2 highest p_t jets

Leptonic top:
b-jets with lowest $d\phi$(jet,lepton),
lepton, E_{tmiss}

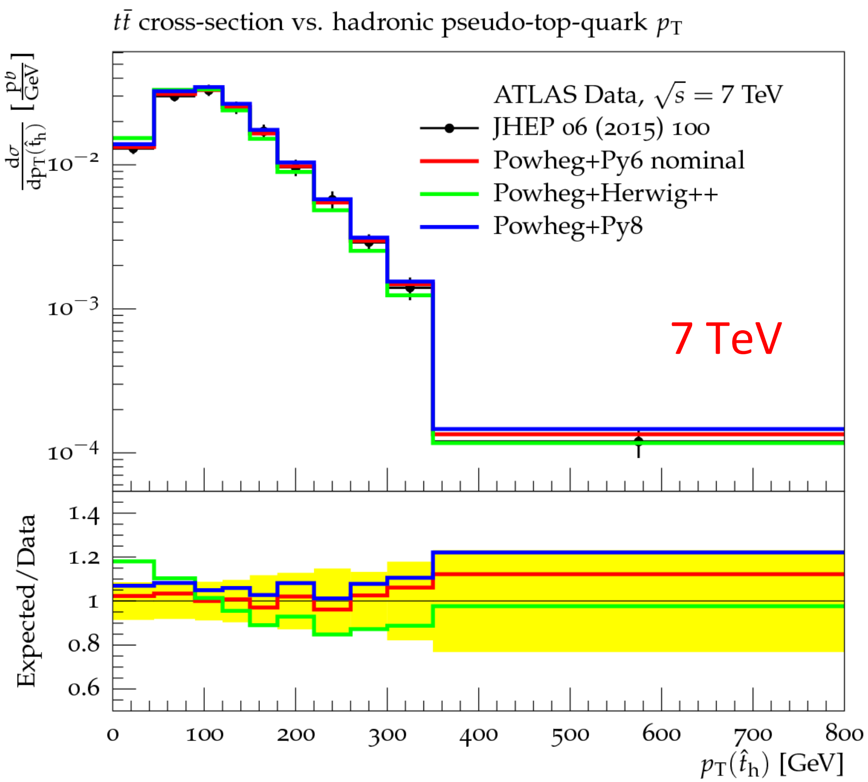


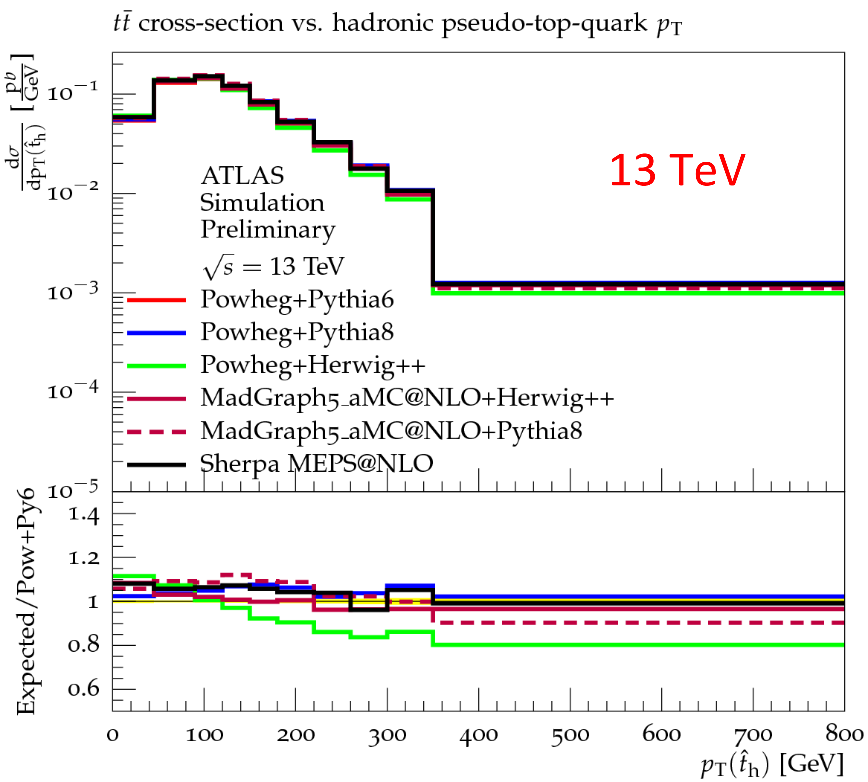


Very good correlation between reco- and particle level

Some shape differences between particle and parton level

Pseudo top pT at various cms energies

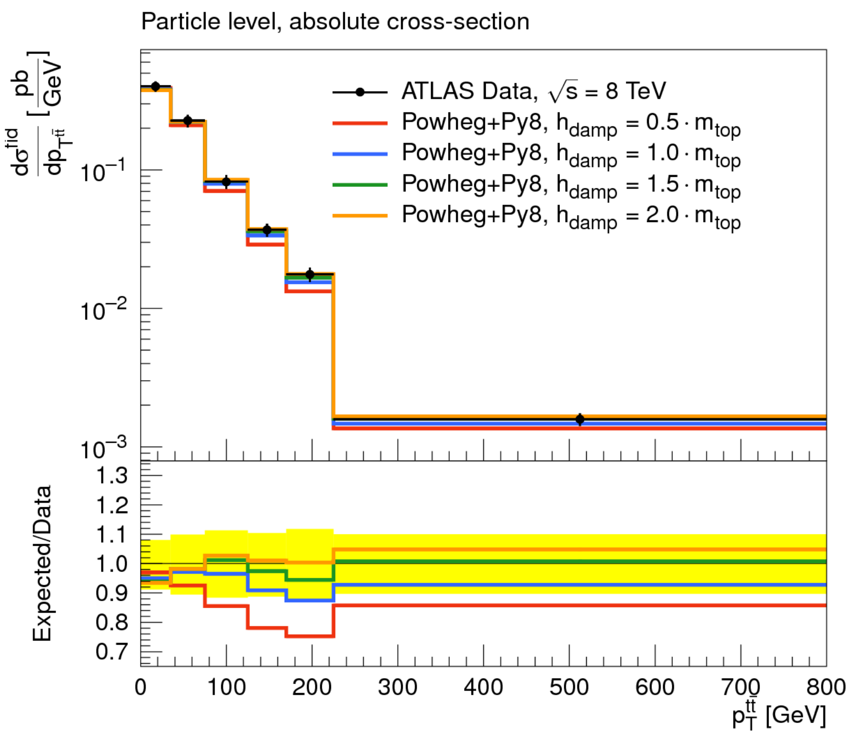


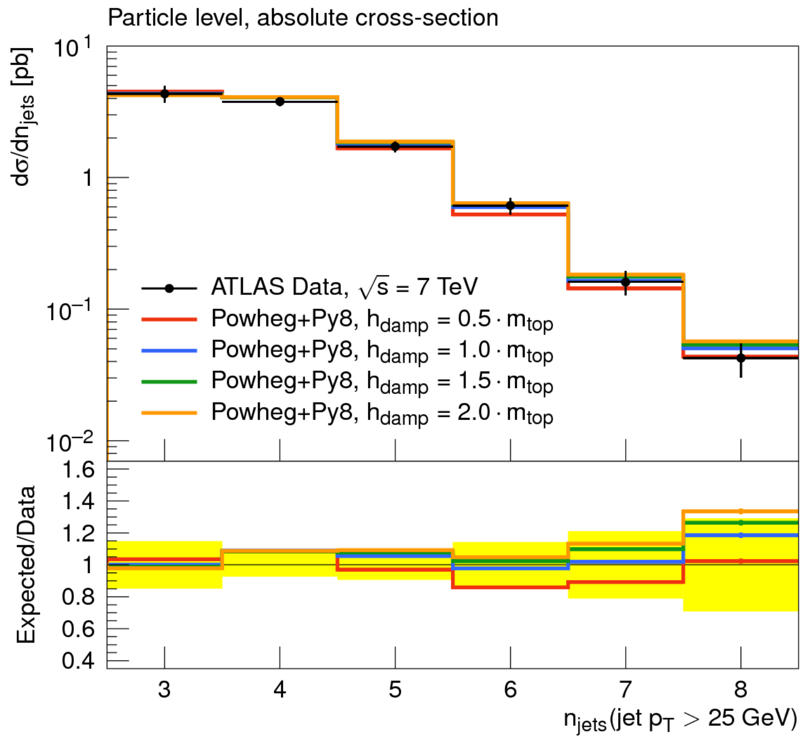


- Overall good description by MC
- More precise data and larger QCD radiation leads to higher discriminating power of 13 TeV data

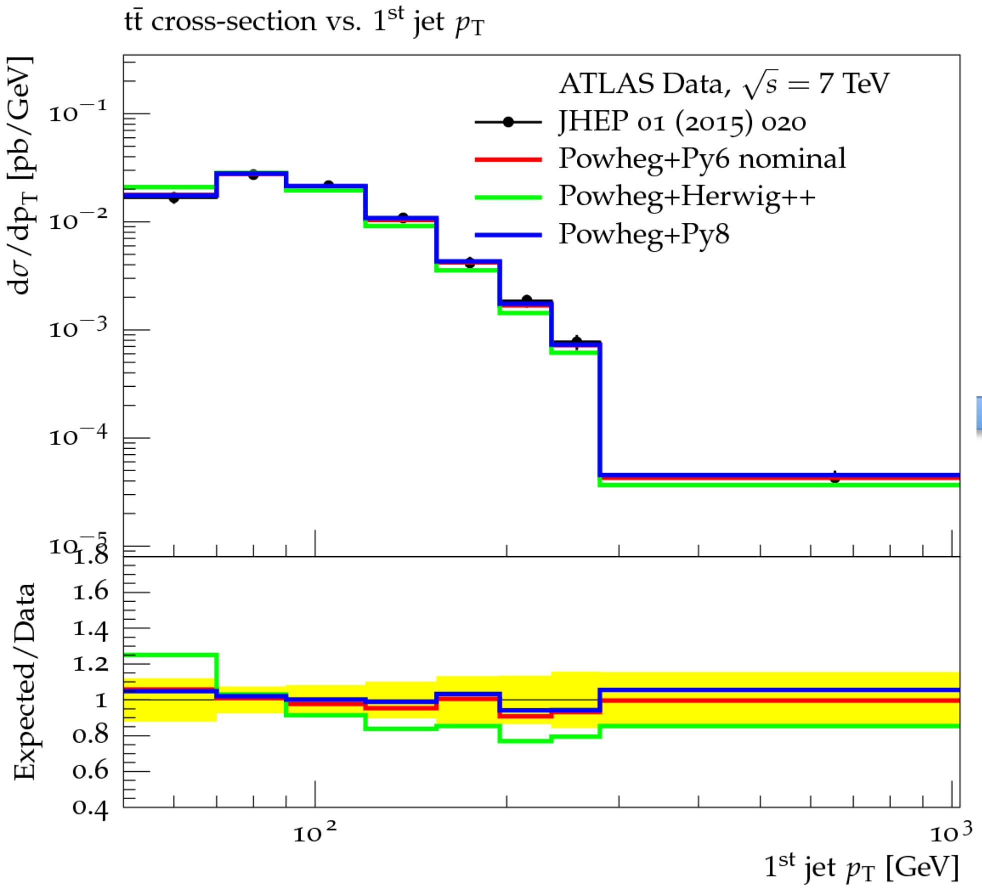
Adjust predictions of PowHeg

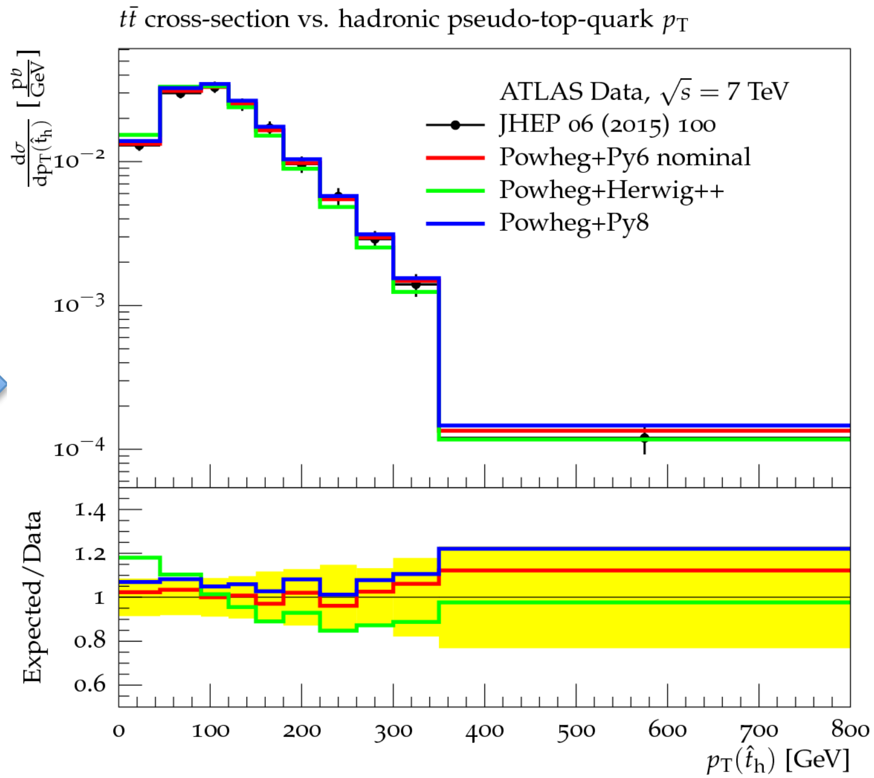
POWHEG: NLO ME for top pair, LO ME for first emission, matched to PS
Model parameter to regulate hardness of first radiation (hdamp)
Measurements are sensitive to the setting of this free model parameter
Best description of tt data with hdamp ~ 1.5 m_{top}





Top decay products vs pseudo top





Some of the effects more visible in

Further reading

Overview:
" QCD Monte-Carlo model tunes for the LHC"

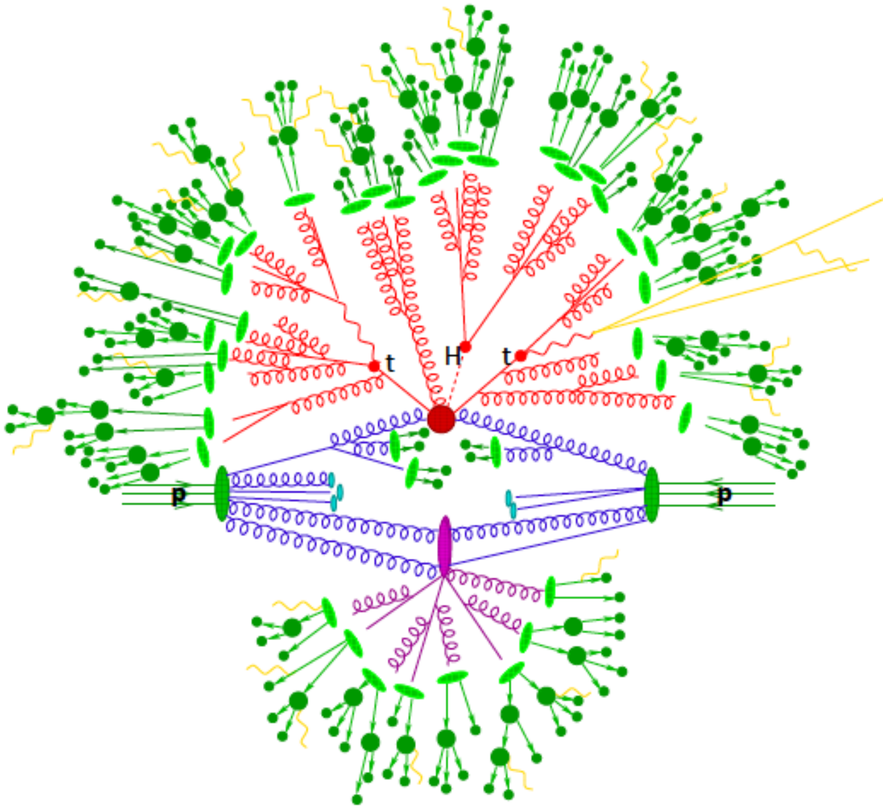
Pythia:
"Tuning Monte Carlo Generators: The Perugia Tunes" arXiv:1005.3457
"Tuning PYTHIA 8.1: the Monash 2013 Tune" arXiv:1404.5630
"Energy Scaling of Minimum-Bias Tunes" arXiv:1103.3649

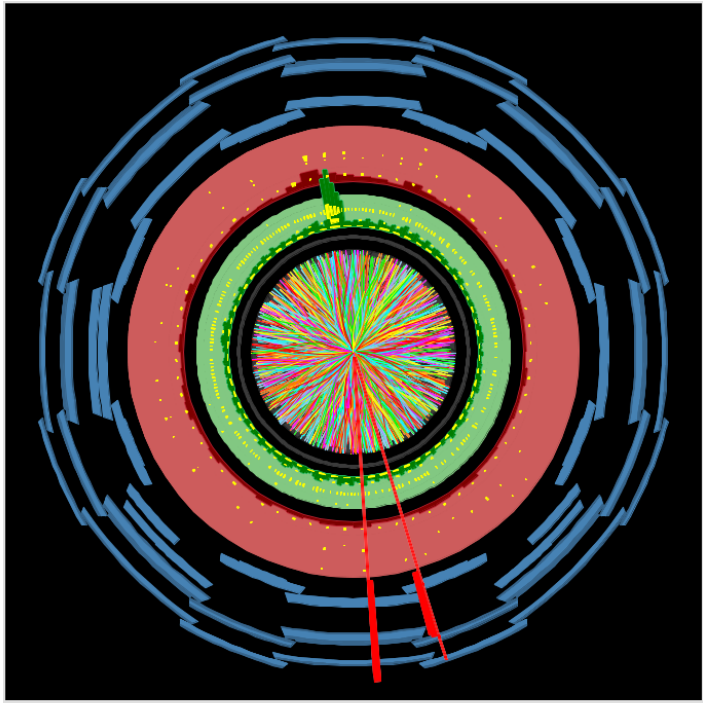
CMS CUET tunes: https://arxiv.org/pdf/1512.00815.pdf

Tuning to multileg generators like alpgen:
"Monte Carlo tuning in the presence of Matching" arXiv:1109.5295

For application to powheg, the following reference introduced the use of vetoed showers:
"Improved Parton Showers at Large Transverse Momenta" arXiv:1003.2384

Summary





- Model independence of measurement key issue for tuning
- Huge set of (unfolded) data available to adjust free parameters of MC Generators
- Precise description of experimental data is essential to perform high precision measurements at LHC

Unfolding

$$\vec{N}_{\text{Signal}} = A\vec{N}_{\text{true}}$$

$$\vec{N}_{\text{true}} = A^{-1}\vec{N}_{\text{Signal}}$$

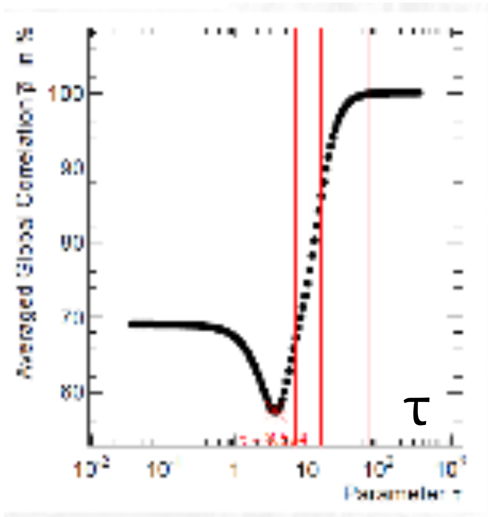
- Ill-posed problem: result is not fully constrained
  - Matrix A can not be unambiguously inverted
  - Data contain no information on structures below detector resolution
  - Can lead to drastic fluctuations (and corresponding anti-correlations between neighboring bins
- Regularization
  - Supplement missing data using assumptions on smoothness of data
  - Add penalty term that gets large for large fluctuations
- One possible approach:
  - Exploit fact that inversion of A is equivalent to minimizing the following expression (where Cov is the covariance matrix)

$$\chi^2 = (\vec{\mathbf{N}} - \mathbf{A}\,\vec{\mathbf{w}})^T \mathbf{Cov}_{\vec{\mathbf{N}}}^{-1} (\vec{\mathbf{N}} - \mathbf{A}\,\vec{\mathbf{w}})$$

  - Introduce penalty term

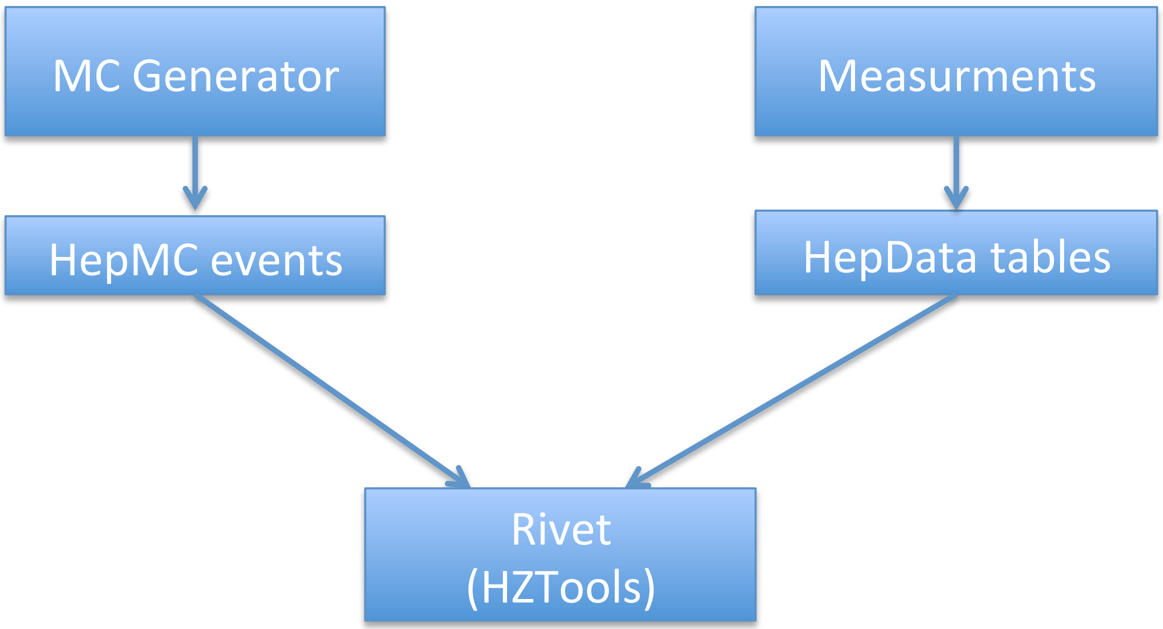
$$\chi^2 = \underbrace{(\vec{\mathbf{N}} - \mathbf{A}\,\vec{\mathbf{w}})^T \mathbf{Cov}_{\vec{\mathbf{N}}}^{-1} (\vec{\mathbf{N}} - \mathbf{A}\,\vec{\mathbf{w}})}_{\chi_A^2} + \tau^2 \cdot \underbrace{K(\vec{\mathbf{w}})}_{\chi_L^2}$$

  - τ is regularization parameter, K(w) is curvature measure
  - Choose τ carefully, e.g. by minimizing global correlation

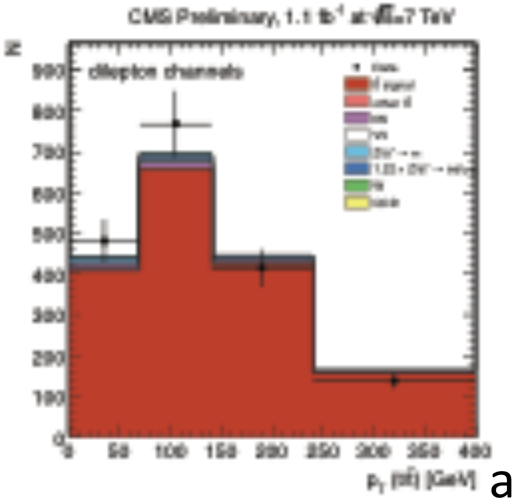


Software & Tools

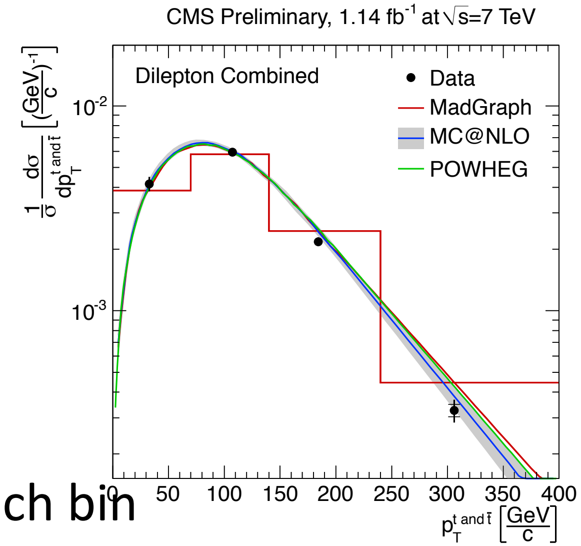
- Rivet (HZTool): analysis libraries for LHC, LEP (HERA) to extract physical observables corresponding to experimental measurements
- MCPLOTS (http://mcplots.cern.ch/) web-accessible repository of theoretical predictions from various MC generators for experimental data
- Professor (Proffit): tuning tool using analytical approximations interfaced to Rivet



Simplest case: Bin-by-bin unfolding



correct measured
Distribution back to
Parton level distribution
(unfolding)



apply efficiency separately in each bin

$$\left(\frac{d\sigma}{dx}\right)_i^{\text{measured}} = \frac{N_i^{\text{data}}}{N_i^{\text{MC}}} \cdot \left(\frac{d\sigma}{dx}\right)_i^{\text{MC}}$$

- Features
  – simple, fast, robust, statistical errors are well defined sqrt(N), biases included in systematics
  – need good description of data, result does not include correlations

Differential Cross Section Measurement

- Measure number of events in many intervals
- Correct for efficiency, acceptance and resolution effects

- Measure bin-averaged cross section in each bins i

$$\frac{d\sigma}{dx} = \frac{N_i}{\Delta x_i \cdot \epsilon \cdot \mathcal{L}_{\text{int}}}$$

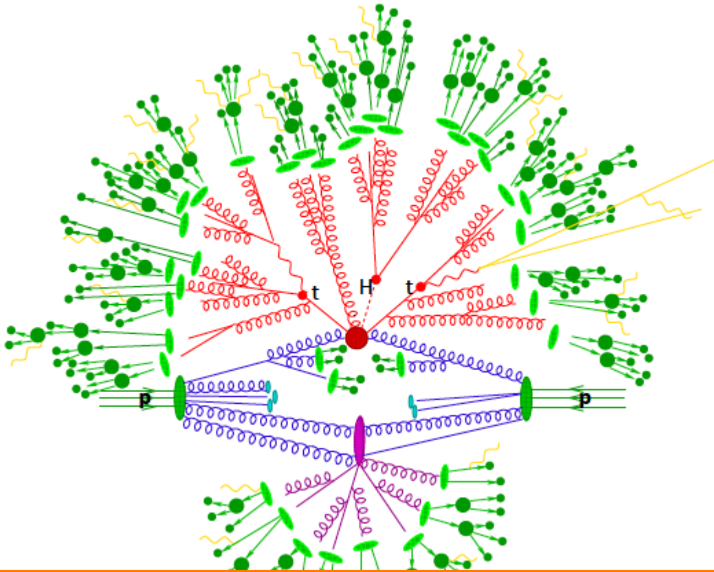
where Δx_i is the width of bin i

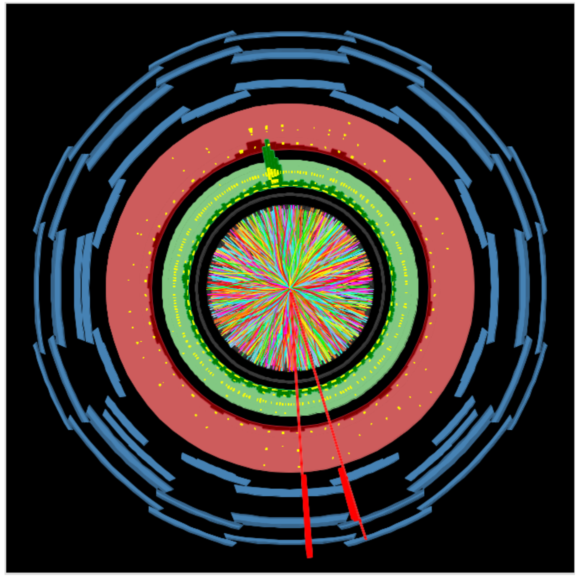
  – Identify bin-averaged cross section with differential cross section. $\frac{\Delta\sigma_i}{\Delta x_i} = \frac{d\sigma(x)}{dx}$
  – Often use theory to perform bin-center correction, e.g. quote measurement at point in x where

- Choice of bins
  – make sure there are enough entries in each bin (minimize statistical errors)
  – make sure there are enough bins (measure shape of distribution)
  – make sure the bin size is large enough w.r.t experimental resolution, i.e. the purity is large

- **Photons**: photons used for final state definitions and for the definition of leptons (electron & muon) should not be from hadron decays. These removes the dependency on the underlying event.
- **Electron**: define 4-momentum from photons and electron within an anti-k_t R=0.1, where leptons (electron & muons) are considered for jet clustering. No isolation condition is imposed. In order to choose prompt leptons from W/Z decay in a way safe for all generators currently under consideration, the parent of the electron is required not to be a hadron or quark (u-b). (Expect that future sanitisation of generator record will remove the need for the quark requirement.)
- **Muon**: define 4-momentum from photons and muon within an anti-k_t R=0.1, where leptons (electron & muons) and photons are considered for jet clustering. No isolation condition is imposed. In order to choose prompt leptons from W/Z decay in a way safe for all generators currently under consideration, the parent of the muon is required not to be a hadron or quark (u-b). (Expect that future sanitisation of generator record will remove the need for the quark requirement.)
- **ETmiss/Neutrinos**: As an event level variable the missing transverse energy is calculated as the 4-vector sum of neutrinos from W/Z--boson decays. Tau decays are included. A neutrino is treated as a detectable particle and is selected for consideration in the same way as electrons or muons, i.e. the parent is required not to be a hadron or quark (u-b). (Expect that future sanitisation of generator record will remove the need for the quark requirement.)
- **Jets**: define with anti-k_t algorithm. Loop over all stable particles excluding the electrons, muons, neutrinos, and photons used in the definition of the selected leptons. This includes non-prompt muons and neutrinos for a proper b-jet energy scale. Use specific R parameter chosen by experiment: R=0.4 for ATLAS and R=0.5 for CMS.
- **b-jets**: A jet is a b-jet if any rescaled B-hadron is included in the jet. A rescaled B-hadron is treated as a stable B-hadron (that does not oscillate or decay to another B-hadron) for which the 4-momentum is scaled down by to the limit of floating point precision and added to the list of particles for jet-clustering as described above. Only B-hadrons with an initial p_T > 5 GeV are considered. This prescription provides an unambiguous way to associate a single jet with a B-hadron.

MC comparison to data





MC generator particles

Particle production in pp collision

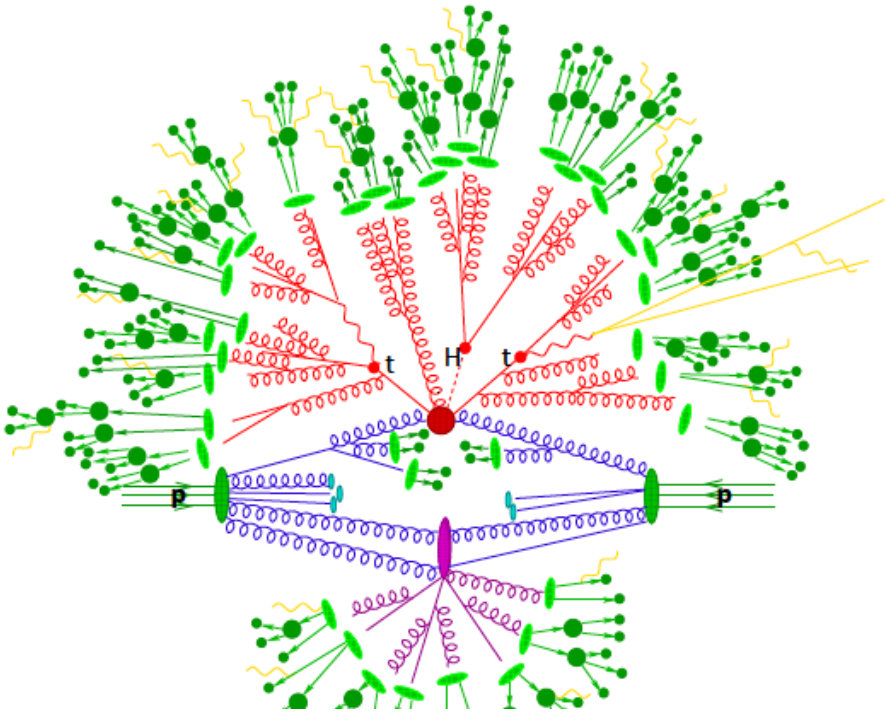
Geant4 simulation of hits in the detector

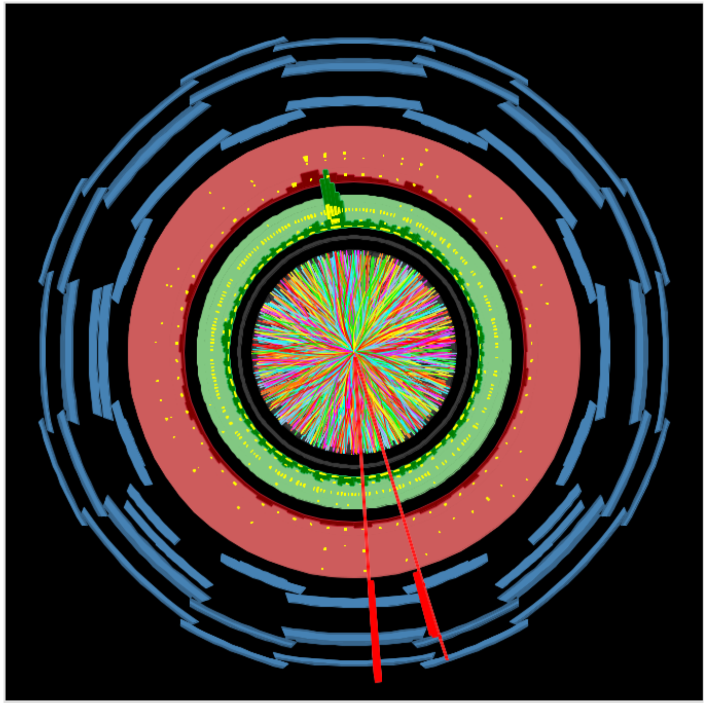
Hits in the detector

Reconstruction & selection

Data-MC comparison

MC comparison to data





MC generator particles

Hits in the detector

Reconstruction & selection

Data-MC comparison

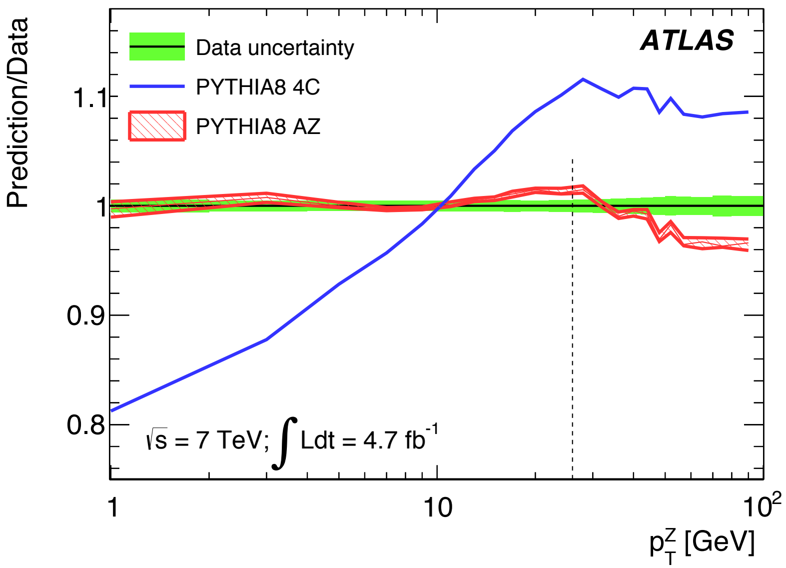
AZ Tune to ISR observables

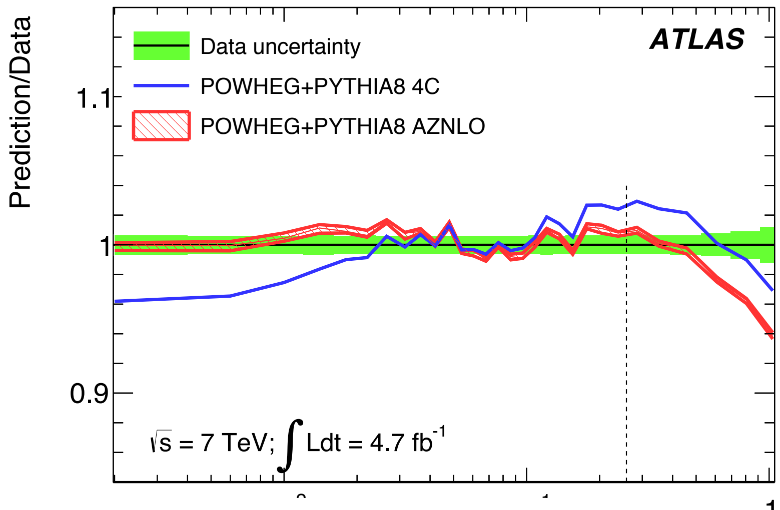
q q -> Z -> e e

Zpt and phi*

Intrinsic kt:
kT of partons inside incoming protons
Fermi motion ~200 MeV
"sum of unresovled effect below shower cut-off"

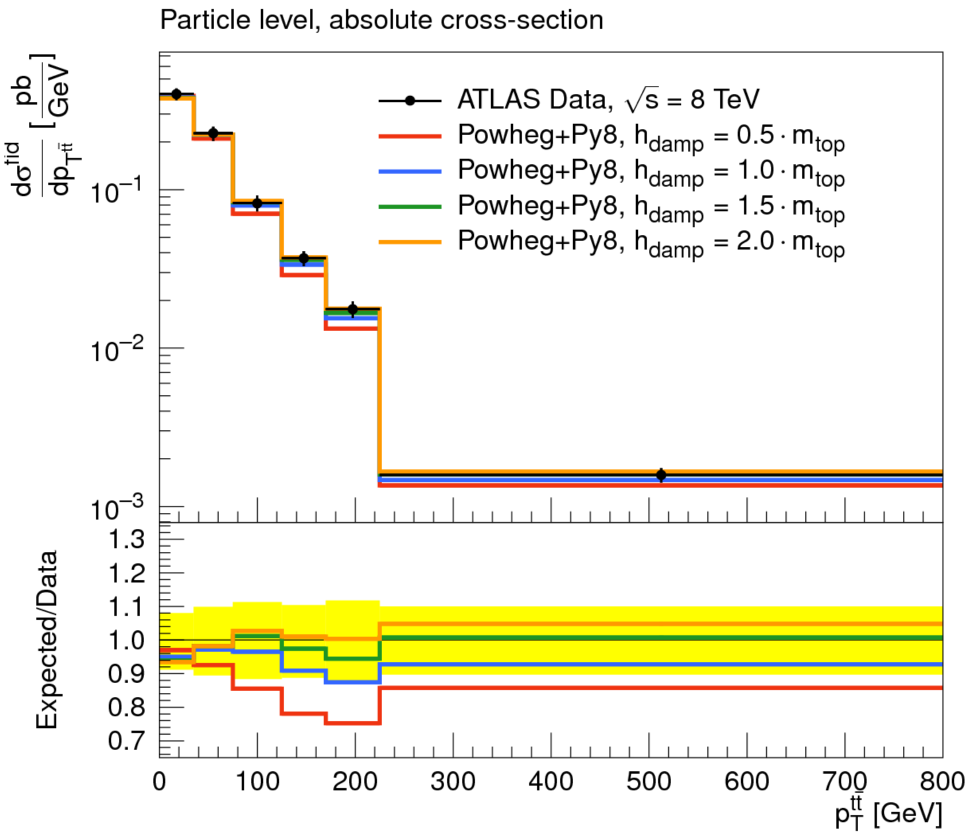
ISR Q_0 cut-off
Alpha_s





$$\phi_\eta^* \equiv \tan(\phi_{acop}/2) \cdot \sin(\theta_\eta^*)$$

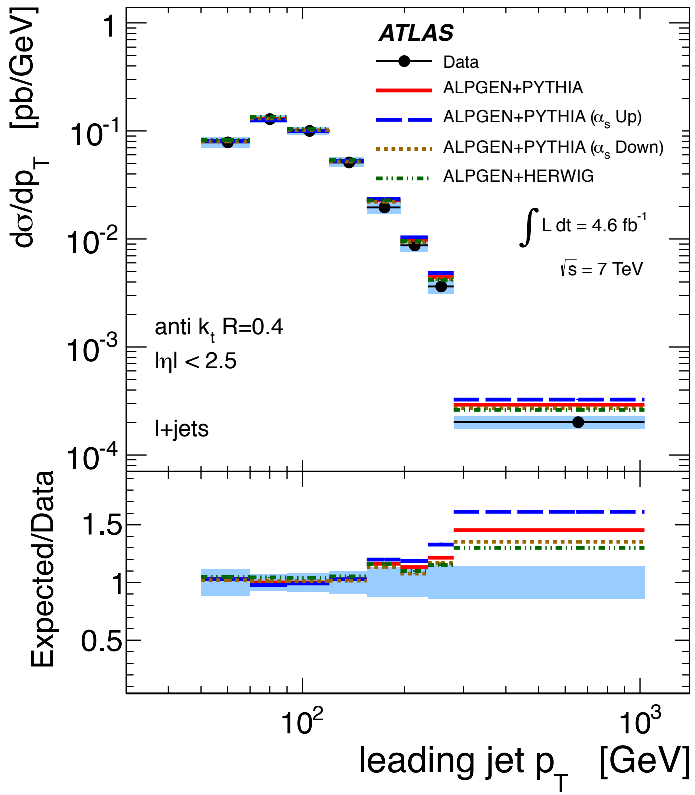
Tuning of hardest allowed emission in ME-PS matching



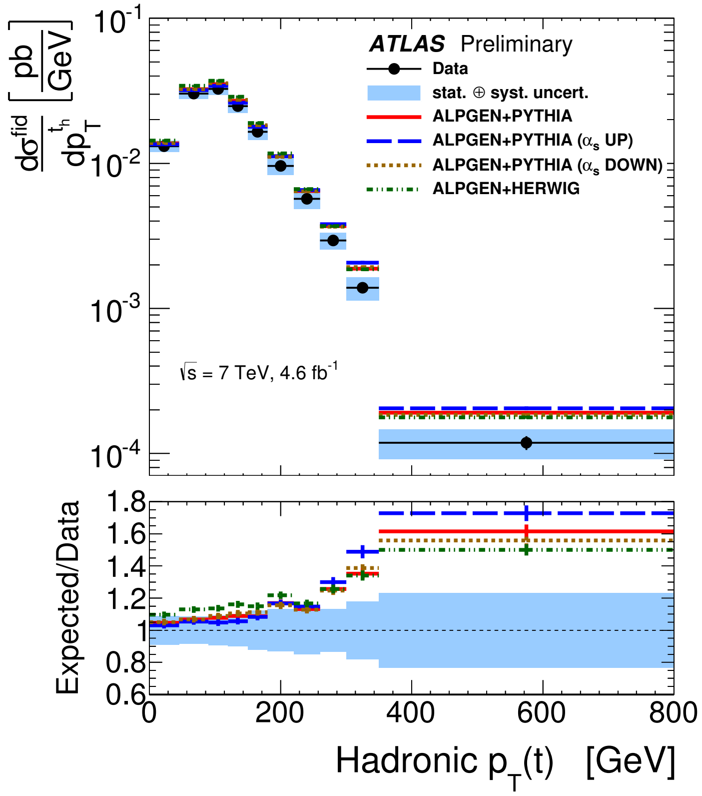
Top pair p_T highly sensitive to QCD radiation

Top decay products vs pseudo top

Fiducial phase space:
>=1 b-jet, 1 lepton, >=3 jets,
1st jet p_t>50 GeV, 2nd jet p_t>35 GeV



Fiducial phase space:
2 b-jets, 1 lepton, >=4 jets



Consistent data – mc description between the observables