Non-Perturbative Aspects of Event Simulation in pp Collisions

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Cnet

MC vs Hadron Collisions

Last Lecture \rightarrow a model that included hard interactions, parton showers, and string fragmentation. Let's apply it to pp collisions!



FIG. 3. Charged-multiplicity distribution at 540 GeV, UA5

 $p_{T\min} = 1.8$ GeV, roughly two-thirds of all events would

Further evidence of additional physics in hadron-hadron collisions

1983: discovery of the "Pedestal Effect" UA1: $p\bar{p}$ at $\sqrt{s} = 540 \text{ GeV}$ Studies of jets with E_T up to 100 GeV

Phys. Lett. B 132 (1983) 214-222

"Outside the [jet], a constant E_T plateau is observed, whose height is independent of the jet E_T . Its value is substantially higher than the one observed for minimum bias events."

In hadron-hadron collisions, **hard jets** sit on **"pedestals"** of increased particle production **extending** far from the jet cores.



What's "Minimum Bias"?

Simple question: what does the average LHC collision look like? First question: how many are there? What is $\sigma_{tot}(pp)$ at LHC ? Around 100mb (of which about half is "inelastic, non-diffractive")



Minimum Bias = Minimal trigger requirement

At least one hit in some simple and efficient hit counters (typically at large η) (Double-sided trigger requirement suppresses "single diffraction")

Dissecting the Pedestal

Today, we call the pedestal "the Underlying Event"





Recall: A uniform (constant) particle density per rapidity unit is just what a string produces ...



but the **height** of the pedestal was much larger than that of **one** string...

Multiple Strings?

Parton-Parton vs Proton-Proton Cross Sections

Total inelastic pp cross section @ 8 TeV* ~ 80 mb (measured by TOTEM)

Compare this to perturbative calculation of $p_{\text{Tmin}} = 0$ scattering cross section (mainly *t*-change gluon exchange; divergent for $p_T \to 0$)



Rati

Interpret to mean that **every** pp collision has **more than one** $2 \rightarrow 2$ QCD scattering with $\hat{p}_{\perp} \leq 4 \text{ GeV}$

*Note: nothing particularly special about 8 TeV; the crossover point would be lower at lower E_{CM} and higher at higher E_{CM}

Physics of the Pedestal

Recall Factorisation: Subdivide calculation

Hard scattering: parton-parton cross section $d\hat{\sigma}$ independent of non-pert. dynamics

x PDF factors $f(x, Q_F^2)$ representing: partitioning of proton into struck **parton** + unresolved **remnant**, at factorisation scale Q_F^2

- Multi-Parton Interactions (MPI)
 - Several QCD 2→2 in one pp collision
 - → need Multi-parton PDFs (PYTHIA, e.g., Sjöstrand & PS JHEP 03 (2004) 053 hep-ph/0402078)

Constructed using **momentum** and **flavour conservation**; goes beyond existing factorisation theorems (though some work on special case Double Parton Scattering)

(More issues such as colour reconnections, saturation, $3 \rightarrow 4$, rescattering, ..., not covered here)



How many?

Naively
$$\langle n_{2
ightarrow 2}(p_{\perp \min})
angle = rac{\sigma_{2
ightarrow 2}(p_{\perp \min})}{\sigma_{
m tot}}$$

If the interactions are assumed ~ independent (naive factorisation) \rightarrow Poisson



$$\mathcal{P}_n = \frac{\langle n \rangle^n}{n!} e^{-\langle n \rangle}$$

Real Life

Colour screening: $\sigma_{2\rightarrow 2}\rightarrow 0$ for $p_{\perp}\rightarrow 0$

Momentum conservation suppresses high-n tail

Impact-parameter dependence

- + physical correlations
- \rightarrow not simple product

Interleaved Evolution in PYTHIA

1987 [Sjöstrand & van Zijl, Phys.Rev.D 36 (1987) 2019]

MPI cast as Sudakov-style evolution in p_T analogous to the one for showers

2005 [Sjöstrand & PS, Eur.Phys.J.C 39 (2005) 129] Interleave MPI & ISR evolutions in one common sequence of pT

→ ISR & MPI "compete" for the available *x* in the proton.

2011 [Corke & Sjöstrand, JHEP 03 (2011) 032] Also include **FSR** in interleaving

2021 [Brooks, PS, Verheyen, SciPost Phys. 12 (2022) 3] Also include **Resonance Decays** in interleaving (VINCIA)



Impact Parameter Dependence



1. Simple Geometry (in impact-parameter plane)

Simplest idea: smear PDFs across a **uniform disk** of size πr_p^2 \rightarrow simple geometric overlap factor ≤ 1 in dijet cross section Some collisions have the full overlap, others only partial \Rightarrow Poisson distribution with different mean $\langle n_{\text{MPI}} \rangle$ at each b

2. More realistic **Proton b-shape** (used by all modern MPI models)

Smear PDFs across a non-uniform disk E.g., Gaussian(s), or **more**/less peaked (e.g., EM form factor) Overlap factor = convolution of two such distributions

 \rightarrow Poisson distribution with different mean <n> at each b "Lumpy Peaks" \rightarrow large matter overlap enhancements, higher <n>

Note: this is an *effective* description. Not the actual proton mass density. E.g., peak in overlap function (\gg 1) can represent unlikely configurations with huge overlap enhancement. Typically use total σ_{inel} as normalization.

MC with MPI vs Hadron Collisions



Characterizing The Underlying Event

There are many UE variables. The most important is $<\Sigma p_T>$ in the "Transverse Region"



"Transverse Region" (TRNS)

Sensitive to activity at right angles to the hardest jets

→ Useful definition of Underlying Event

Min-Bias VS Underlying Event

Tautology:

A jet trigger provides a bias (→subsample of minimum-bias)

Pedestal effect:

Events with a hard jet trigger are accompanied by a higher plateau of ambient activity

MPI: interpreted as a biasing effect. Small pp impact parameters → larger matter overlaps → more MPI → higher chances for a hard interaction



Colour Space in Hadron Collisions



Colour Correlations

Each MPI exchanges colour between the beams

The colour flow determines the hadronizing string topology



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Colour Connections



Colour Reconnections?

Multi-Parton Interactions + Colour coherence \rightarrow Multiplicity \neq NMPI ?



Hadronization — with MPI



~ the equivalent of "independent fragmentation" for MPI

→ Each MPI hadronizes independently of all others

"Leading Colour"

Colour Reconnections (CR)

With Colour Reconnections MPI hadronize collectively But how do we know which partons should be confined with which?



Confinement in LHC Collisions

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Lelefer

MP

High-energy pp collisions — with ISR, MPI, and Beam Remnants Final states with very many coloured partons Who gets confined with whom?

"OCD Colour Reconnection" Model: [Christiansen & PS JHEP 08 (2015) 003] Stochastically sample ~ all possibilities E.g.: random triplet charge has 1/9 chance to be in singlet state with random antitriplet: $3 \otimes \overline{3} = 8 \oplus 1$ $3 \otimes 3 = 6 \oplus \overline{3}$; $3 \otimes 8 = 15 \oplus 6 \oplus 3$

 $8 \otimes 8 = 27 \oplus 10 \oplus \overline{10} \oplus 8_S \oplus 8_A \oplus 1$

Choose between allowed string configurations: smallest world-sheet area (a.k.a. "string-length" minimization)

*): in this context, QCD CR simply refers to an ambiguity beyond Leading N_C, known to exist. Note the term "CR" can also be used more broadly to incorporate further physics concepts.

How to confront with measurements?

Can't measure n_{MPI} directly

Use number of particles produced ~ rough indicator of how much colour gets kicked around

 \implies study event properties as a function of "N_{ch}" = N_{tracks}

Different models/tunes

Predict different number of charged particles "per" MPI

But all predict a strong correlation → useful indicator



Consequences of CR: <p_>(nch)



+ New junction-type CR



What a strange world we live in, said Alice

We also know ratios of strange hadrons to pions strongly increase with event activity





→ Non-Linear String Dynamics?

$MPI \implies lots$ of coloured partons scattered into the final states

Count **# of flux lines** crossing y = 0 in pp collisions (according to PYTHIA): Multiplets (y=0, pp 7 TeV)



LEP

I EP

Particle Composition: Impact on Jet Energy Scale



ATLAS PUB Note ATL-PHYS-PUB-2022-021 29th April 2022



Dependence of the Jet Energy Scale on the Particle Content of Hadronic Jets in the ATLAS Detector Simulation

The dependence of the ATLAS jet energy measurement on the modelling in Monte Carlo simulations of the particle types and spectra within jets is investigated. It is found that the hadronic jet response, i.e. the ratio of the reconstructed jet energy to the true jet energy, varies by $\sim 1-2\%$ depending on the hadronisation model used in the simulation. This effect is mainly due to differences in the average energy carried by kaons and baryons in the jet. Model differences observed for jets initiated by *quarks* or *gluons* produced in the hard scattering process are dominated by the differences in these hadron energy fractions indicating that measurements of the hadron content of jets and improved tuning of hadronization models can result in an improvement in the precision of the knowledge of the ATLAS jet energy scale. Variation largest for gluon jets For $E_T = [30, 100, 200]$ GeV Max JES variation = [3%, 2%, 1.2%]

Fraction of jet E_T carried by baryons (and kaons) varies significantly

Reweighting to force similar baryon and kaon fractions

Max variation → [1.2%, 0.8%, 0.5%]

Significant potential for improved Jet Energy Scale uncertainties!

Motivates Careful Models & Careful Constraints

Interplay with advanced UE models In-situ constraints from LHC data Revisit comparisons to LEP data



Extra Slides







PART 2

Tuning & Validation

Tuning: **PROFESSOR** — a powerful tool for (semi)automated tuning

Run generator and fill histograms

Inspired by idea pioneered by DELPHI (Hamacher et al., 1995): Bin-wise interpolation of MC response and χ^2 minimization 2^{nd} -order polynomials account for parameter correlations.



Random sampling: N parameter points in *n*-dimensional space

Modern Python Package with much more functionality, tutorials, etc. https://professor.hepforge.org/

procedure Professor Tuning

polynomial)



2 **3** For each bin: use N points to fit interpolation $(2^{nd} \text{ or } 3^{rd} \text{ order})$ • Construct overall (now trivial) $\chi^2 \approx \sum_{bins} \frac{(interpolation-data)^2}{error^2}$ In and Numerically *minimize* pyMinuit, SciPy

Caveat 1: Tensions vs Incompatibilities ?

Physics Model may not be able to simultaneously agree with all measurements

Not immediately a concern. Consider overall physics/consistency ↔ your priorities.

Physics Model may be unable to agree with (some part of) a given measurement

Fit reacts by desperately trying to reduce order-of-magnitude differences in bins it shouldn't have been asked to fit in the first place

At cost of everything else \blacktriangleright total garbage.

Choose measurements carefully

Within context of physics model \longleftrightarrow domain of applicability

This can also apply to *bins* of a histogram, e.g., if part of a measurement goes outside domain of validity of theory model

E.g., professor allows to put zero (or very small) weights for some bins

Consider whether you should effectively "give up" on some measurements

Caveat 2: Sensitivities and Observable Hierarchies

For each observable and/or MC parameter you want to consider: What is/are the most salient MC parameter(s) which **that** observable is sensitive to PROFESSOR can help with this → sensitivity and correlation analyses What is a **full set of observables** that **span** constraints on those parameters?

Are some of those observables/parameters more important than others? Do some parameters control larger aspects of the modelling → Cross checks. Are some observables more important to you than others? → Weightings.

Example: a measurement reveals the kaon yield is too low in the MC

You can increase the production of *all* particles, including kaons

Or you could increase just the strangeness fraction keeping the total constant

If you don't know and don't think about this, you risk tuning to agree with kaons while mistuning agreement on the overall level of particle production. Is that what you want?

ightarrow include an observable sensitive to the total number of particles (or kaon fraction)

Caveat 3: Overfitting

Very precisely measured data points can generate large χ^2 values Even if MC gets within what one would naively consider "reasonable" agreement

Fit reacts by sacrificing agreement elsewhere (typically in tails) to improve χ^2 in peaks.

Still bad overall fit, typically not spanning uncertainties (only on one side)

My recommendation:

Include a "sanity limit" (e.g., 5%) "theory uncertainty"

► Fit not rewarded (much) for improving agreement beyond that point. More freedom in tails

Also tends to produce $\chi^2_{5\%}$ values ~ unity \rightarrow better uncertainty bands?

Some Helper Tools

Wouldn't it be nice if there was a tool:

- That could automatically detect correlations between parameters and observables.
- And tell you which "groups" they fall into naturally : which parameter sets you should ideally tune together, and which are more nicely factorised.
- This is (at least partly) what the tool AutoTunes does Bellm, Gellersen, Eur.Phys.J.C 80 (2020) I won't have time to discuss that today, but I think it looks promising I encourage you to study it and use it

You may also be interested in Apprentice Krishnamoorthy et al., EPJ Web Conf. 251 (2021) 03060

Variance reduction to semi-automate how to weight observables & bins



ABOUT PLOTS - COMPARISON - LHC@HOME

MCPLOTS

Online repository of Monte Carlo plots compared to experimental data



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Parameters (in PYTHIA): FSR pQCD Parameters

Matching



Additional Matrix Elements included?

At tree level / one-loop level? Using what matching scheme?

a_s(m_Z)



The value of the strong coupling

In PYTHIA, you set an effective value for $\alpha_s(m_Z^2) \Leftrightarrow$ choice of k in $\alpha_s(kp_{\perp}^2)$



Renormalization Scheme and Scale for α_s

1- vs 2-loop running, MSbar / CMW scheme, choice of k in $\alpha_s(kp_{\perp}^2)$, cf





Ordering variable, coherence treatment, effective $1 \rightarrow 3$ (or $2 \rightarrow 4$), recoil strategy, ...

Branching Kinematics (z definitions, local vs global momentum conservation), hard parton starting scales / phase-space cutoffs, masses, non-singular terms, ...

Parameters (in PYTHIA): String Tuning





Fragmentation Function

The "Lund *a* and *b* parameters" Or use *a* and $\langle z \rangle$ instead (less correlated) A. Jueid et al., JCAP 05 (2019) 00 + $\Delta a_{\text{diquark}}$ for baryons

p_{T} in string breaks



Scale of string-breaking process Shower cutoff and $\langle p_{\perp} \rangle$ in string breaks





Meson Multiplets

Mesons

Strangeness suppression, **Vector/Pseudoscalar**, η , η' , ...

Baryon Multiplets

Baryons



Baryon-to-meson ratios, **Spin-3/2 vs Spin-1/2**, "popcorn", colour reconnections (junctions), ... ?

Parameters (in PYTHIA): Initial-State Radiaton

Matching & Merging



Additional Matrix Elements included?

At tree level / one-loop level? What matching scheme?



Size of Phase Space Starting scale

Relation between Q_{PS} and Q_{F} (Vetoed showers? Suppressed? cf matching)

Initial-Final interference

I-F colour-flow interference effects (eg VBF & Tevatron $t\bar{t}$ asym) & interleaving



Coherence

Value and running of the strong coupling Governs overall amount of radiation (cf FSR)

"Primordial kT"



A small additional amount of "unresolved" kT Fermi motion + unresolved ISR emissions + low-x effects?

Minimum-Bias & Underlying Event

Number of MPI



Infrared Regularization scale $p_{\perp 0}$ for the QCD 2→2 (Rutherford) scatterings used for multiple parton interactions

 \rightarrow average number of MPI, sets size of overall UE activity

Note: strongly correlated with choice of PDF set! (low-x gluon)

Pedestal Rise



Proton transverse mass distribution → difference between central (more active) vs peripheral (less active) collisions

Strings per Interaction



Color correlations between multiple-parton-interaction systems (aka colour *reconnections* — relative to LC)

 \rightarrow shorter or longer strings \rightarrow less or more hadrons per MPI

Affect $< p_T > vs N_{ch}$ balance: High CR \rightarrow fewer particles, each carrying more p_T



Evolution of UE, $\langle dN/d\eta \rangle$, ... with collider CM energy

Cast as energy evolution of p_{TO} parameter.

IR Safe Observables: Sensitivity to Hadronization Parameters

PYTHIA 8 (hadronization on) Vs (hadronization off)

Important point: These observables are IR safe \rightarrow minimal hadronisation corrections Big differences in how sensitive each of these are to hadronisation & over what range



The shaded bins provide constraints for the non-perturbative tuning stage. You want your hadronization power corrections to do the "right thing" eg at low Thrust.

Hadronization Corrections: Fragmentation Tuning

Now use infrared **sensitive** observables - sensitive to hadronization + first few bins of previous (IR safe) ones

momentum do they carry? 91 GeV ee Z (hadronic 91 GeV ee Z (hadronic dσ/dξ_p Charged multiplicity (particle-level, charged) Log of scaled momentum (OPAL All events) b/1 $\xi_p = \ln$ **Multiplicity Distribution** 10 of Charged Particles (tracks) Momentum Distribution at LEP ($Z \rightarrow hadrons$) of Charged Particles (tracks) at LEP ($Z \rightarrow hadrons$) 10-2 ALEPH 1996 S3486095 OPAL 1998 S3780481 hia 6.426 Pythia 8.162 Sherna 1.4.0 2.5.2, Pythia 6.426, Pythia 8.162, Sherpa 1.4.0, Vincia 1.0.2

And how much

How many hadrons do you get?

Longitudinal FF parameters *a* and *b*.

-5

dN/dN

₹ 10⁻¹

10

10

10

10-5

Transverse p_T broadening in string breaks (curtails high-N tail, and significantly affects event shapes)

Further parameter a_{diquark} requires looking at a baryon spectrum

 $<N_{ch}(M_Z)> \sim 21$

40

N_{ch}

20

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Practical Example: Uncertainties on Dark-Matter Annihilation Spectra

Based on A. Jueid et al., <u>1812.07424</u> (gamma rays, eg for GCE) and <u>2202.11546</u> (antiprotons, eg for AMS) + <u>2303.11363</u> (all)

Compare different generators?

- E.g., HERWIG PYTHIA
- Problem: tuned to ~ same data

Difference not guaranteed to span genuine uncertainties





Practical Example: Uncertainties on Dark-Matter Annihilation Spectra

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Same done for antiprotons, positrons, antineutrinos

Tables with uncertainties available on request. Also the spanning tune parameters of course.

Main Contact: adil.jueid@gmail.com



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Meson and Baryon Rates and Ratios

From PS et al., "Tuning PYTHIA 8.1: the Monash 2013 Tune", Eur.Phys.J.C 74 (2014) 8



ISR + Primordial kT



Controlling for Process Dependence!

Note: these distributions rely on Pythia's "Power Showers"





→ we should ensure we do MECs / matching / merging if we want to use them (or something equivalent to that.)

Underlying Event

Same thing as before: how many particles do you get? And how much p_T do they carry?

UE - LHC from 900 to 7000 GeV - ATLAS



As you trigger on progressively higher p_T , the entire event increases ...

... until you reach a plateau ("max-bias") also called the "jet pedestal" effect **Interpreted as impact-parameter effect** Qualitatively reproduced by MPI models

Relative size of this plateau / min-bias depends on pT0, PDF, and b-profile

"Toward"

Interplay between MPI and PDF set



"The Tyranny of Carlo" [J. D. Bjorken, ca. 1990]

"Another change that I find disturbing is the rising tyranny of Carlo. No, I don't mean that fellow who runs CERN [Rubbia], but the other one, with first name Monte.

The simultaneous increase in detector complexity and in computation power has made simulation techniques an essential feature of contemporary experimentation. The MC simulation has become the major means of visualization of not only detector performance but also of physics phenomena. **So far so good.**

But it often happens that the physics simulations provided by the MC generators carry the authority of data itself. They look like data and feel like data, and if one is not careful they are accepted as if they were data. **All Monte Carlo codes come with a GIGO* warning label**. But that warning label is just as easy for a physicist to ignore as that little message on a packet of cigarettes is for a chain smoker to ignore. I see nowadays experimental papers that claim agreement with QCD (translation: someone's simulation labeled QCD) and/or disagreement with an alternative piece of physics (translation: an unrealistic simulation), without much evidence of the **inputs into those simulations**."

Treat Tuning & Validation Studies with **same scientific rigour** as any other scientific endeavour

Event Simulation — Summary

Physics

Separation of time scales > Factorizations

Maths

 \rightarrow Can split big problem into many (nested) pieces + make random choices (MC)² ~ like in nature

 $\mathcal{P}_{\text{event}} = \mathcal{P}_{\text{hard}} \otimes \mathcal{P}_{\text{dec}} \otimes \mathcal{P}_{\text{ISR}} \otimes \mathcal{P}_{\text{FSR}} \otimes \mathcal{P}_{\text{MPI}} \otimes \mathcal{P}_{\text{Had}} \otimes \dots$



Hard Process & Decays:

Use process-specific (N)LO matrix elements (e.g., $gg \rightarrow H^0 \rightarrow \gamma\gamma$) \rightarrow Sets "hard" resolution scale for process: Q_{HARD}

ISR & FSR (Initial- & Final-State Radiation):

Driven by differential (e.g., DGLAP) evolution equations, dP/dQ^2 , as function of resolution scale; from Q_{HARD} to $Q_{HAD} \sim 1 \text{ GeV}$

MPI (Multi-Parton Interactions)

Protons contain lots of partons \rightarrow can have additional (soft) parton-parton interactions \rightarrow Additional (soft) "Underlying-Event" activity

Hadronisation

Non-perturbative modeling of partons \rightarrow hadrons transition Strings or clusters; followed by hadron and τ decays

corrections

Final Words

MCs *can* be treated as black boxes, without knowing what's in them.

Best Case: Limited Sophistication

Worst Case: Not your lucky day

The key to successful Monte Carlo:

In the words of Kenny Rogers

Knowing what to throw away Knowing what to keep

> Kenny Rogers "The Gambler", first recorded in 1978 Same year as the first version of PYTHIA (JETGEN)

