Event generators for collider physics

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Introduction

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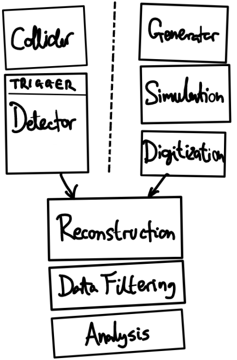
"Evgen" is simulation of the fundamental particle-collision process

- Ubiquitous in HEP, from experiment design to interpretation
- I'll focus on fully differential "shower+hadronisation" gens (SHGs): those that make "realistic" events that can be fed to a detector simulation
- These are serious theory tools ⇒ the link between "hardcore theory" and experiment. Precision (and CPU cost) have rocketed in the last decade
- But often treated as *black boxes*…rarely a good idea. A little extra understanding can go a long way, so let's see what we can do!



Early excuse: I'm more a user than developer. **Apologies in advance to *real* experts!**

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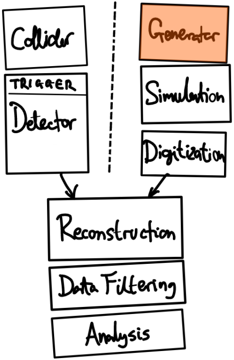

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What is an event generator?

- "Event generator" is an overloaded phrase: many pheno people refer to partonic MC integrators (e.g. MCFM, TOP++, NLOJET++, …) as event generators. And "MC" includes Geant4!
- For experiment purposes a real EG produces *exclusive* events
  - Realistic final particle multiplicities & composition, cf. real data
  - Fortunately HEP final-states *really* can be described in full detail
- Correlations are not easily fakeable, e.g. from sampling data distributions: *microscopic models* produce best and most richly structured phenomena
  - i.e. event generators are based on fundamental QFT
  - but *approximately*: can't explicitly calculate full-multiplicity processes
- Since QCD is the strongest force, QCD effects usually dominate MC physics. But this is changing, cf. precision era and large EW corrections for future colliders, for both lepton and hadron beams.

Shower & hadronisation event generators (SHGs)

What's an SHG good for? Depends who you ask!

- **Experimentalists:** design of colliders, detectors & analyses, background estimation, signal estimation, pile-up estimation, unfolding. . . ∼**everything!**
- **Theory/pheno:** dressing parton level calculations to make them more realistic ("easily" include effects that aren't the focus of the study e.g. decays or UE); constraining BSM models by "recasting" experimental data
- **Generator authors:** understanding (how to work with) QCD – both perturbative and non-perturbative; enabling both the above

SHGs often take in partonic events via *LHE format* (though this is evolving), and output full particle-level events via *HepMC format(s)*

A selective list

- **Partonic subprocess generators (used as SHG input via LHE):**
  - Multi-leg LO: MadGraph5, Sherpa, ~~AlpGen~~
  - NLO (+ multileg): POWHEG-BOX, Sherpa, OpenLoops, MadGraph5-aMC@NLO, MCFM
  - Specialist processes: HEJ, Prophecy4f, WHiZard, Protos, HEJ

- **Main general-purpose event gens:**
  - C++: Sherpa, Herwig 7, Pythia 8
  - FORTRAN: ~~FHerwig~~ and ~~FPythia~~

- **Afterburners:**
  - EvtGen, Photos, Tauola, ~~Jimmy~~

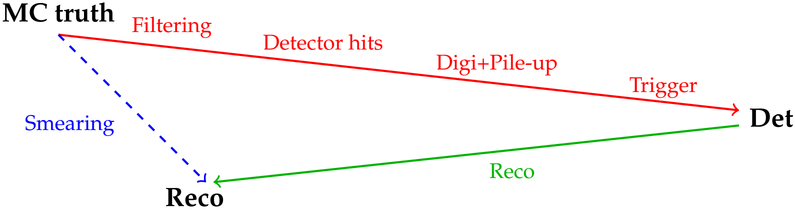
- **Specialist all-in-one:**
  - Min bias & air showers: PHOJET, EPOS, QGSJET, SYBILL
  - Heavy ion: HIJING, HYDJET, Starlight, Angantyr

- **Utilities:**
  - LHAPDF, HepMC

Evgen in experiment data-processing

Typical experimental use of generators is to feed their output into a detector sim, e.g. based on Geant 4.

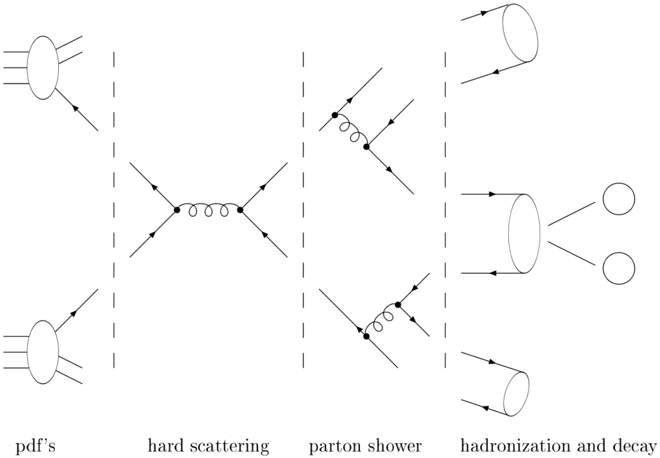
Then apply the same reconstruction + analysis as for data:



The generator bit of this chain was long considered “free” – few programs with few modes, and CPU/memory requirements *much* less than detector geometry + B-field stepping + material interaction + secondaries. Not true these days! ↗ ↗

Generator capabilities, complexity & CPU demands greatly increased.

Anatomy of an SHG



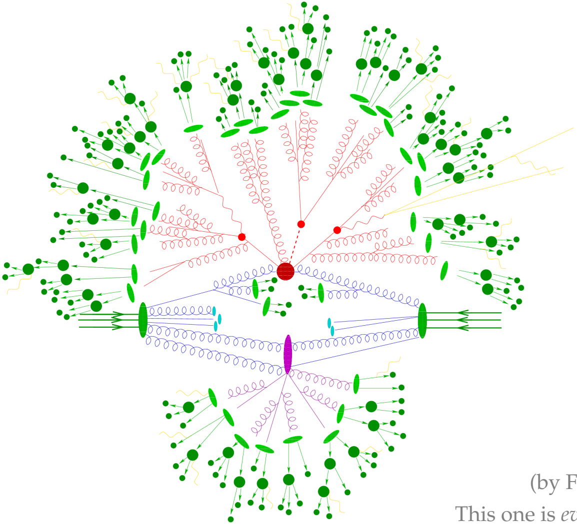
ME
Shower
Hadronisation
Decays

ISR
UE
PDFs
BSM,
diffraction,
$\tau, \gamma, B \ldots$

This diag ignores UE and ISR

Anatomy of an SHG

Or, alternatively…

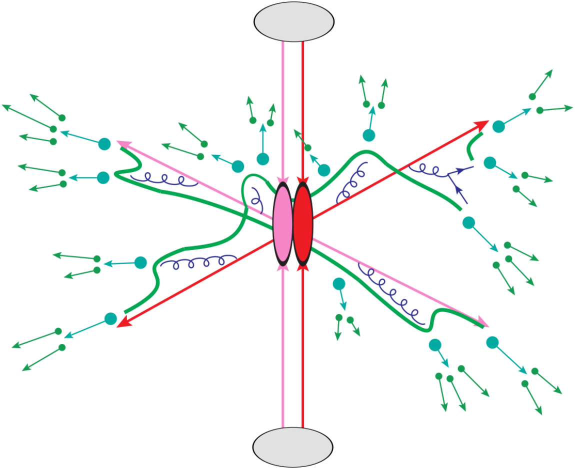


(by Frank Krauss)

This one is *everywhere*…

Anatomy of an SHG

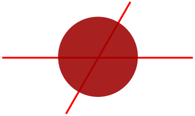
Or. . .



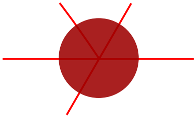
(by Stefan Prestel)

Matrix elements

SHG step-by-step



SHG step-by-step



Matrix elements and phase-space

Cross-sections for a scattering subprocess $ab \to n$ computed in collinear factorization:

$$
\begin{aligned}
\sigma &= \sum_{a,b} \iint_0^1 \mathrm{d}x_a \mathrm{d}x_b \int f_a^{h_1}(x_a, \mu_F)\, f_b^{h_2}(x_b, \mu_F)\, \mathrm{d}\hat{\sigma}_{ab\to n}(\mu_F, \mu_R) \\
&= \sum_{a,b} \iint_0^1 \mathrm{d}x_a \mathrm{d}x_b \int \mathrm{d}\Phi_n\, f_a^{h_1}(x_a, \mu_F)\, f_b^{h_2}(x_b, \mu_F) \\
&\qquad \times \frac{1}{2\,\hat{s}} |\mathcal{M}_{ab\to n}|^2 (\Phi_n; \mu_F, \mu_R)\,,
\end{aligned}
$$

This is the core of all event generation: a combined *integral* of PDFs and partonic matrix element over phase space in $x_{a,b}$ and Φ.

The "MC" comes in because the integral is done by Monte Carlo sampling in $4(n-1)+2$ phase space dimensions: error reduces as $\sqrt{\text{samples}}$, rather than degrading with N_{dim}.

ME integration & generation

Event generation is preceded by an integration phase to evaluate total cross-section and map the $\mathrm{d}\hat{\sigma}$ structure in ME phase-space

Naïve sampling doesn't get far: easy to spend all CPU on *atypical points* which are dwarfed by a lucky strike on the typical set (if you're lucky!) NLO $V+\geq 2j$ sampling = LHC #1 MC performance challenge

A better strategy:

- Jacobian-transform phase space to remove divergent structures;
- But there are *many* characteristic divergences in matrix elements ⇒ multi-channel integration: one per divergence, cf. MG5
- Use standard sampling techniques, or adaptive sampling algorithms — even ML

Integration can take *months*! Massively parallel computations becoming normal. Typically save integration results as "gridpack" files for batched event generation.

(Far) beyond LO

We are long past the point where SHGs only handle lowest-order partonic subprocesses (sometimes enhanced with LO *ME corrections* for the first parton shower emission).

Extra partonic emissions at tree-level increase the final state multiplicity and change the event kinematics directly. Automated by LO *merging and matching schemes* like MLM, CKKW(-L), etc.

Going beyond tree-level is more involved. An NLO cross-section has 3 parts:

$$\mathrm{d}\sigma^{\mathrm{NLO}} = \mathrm{d}\tilde{\Phi}_n \left[\mathcal{B}(\tilde{\Phi}_n) + \alpha_\mathrm{s}\mathcal{V}(\tilde{\Phi}_n)\right] + \mathrm{d}\tilde{\Phi}_{n+1}\alpha_\mathrm{s}\mathcal{R}(\tilde{\Phi}_{n+1})$$

But infrared divergences occur in both the $\mathcal{R}$eal emission and $\mathcal{V}$irtual correction parts – i.e. in different Φ dimensionalities.

Bloch–Nordsieck / KLN theorems: for infra-red-safe observables, these divergences must cancel. cf. ME squaring

(Far) beyond LO

Subtraction: use universal splitting kernel $\mathcal{S}$ which encodes real emission divergence structure so $\mathcal{R} - \mathcal{B} \otimes \mathcal{S}$ is finite → computable:

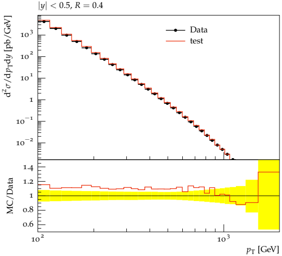
$$\sigma^{\mathrm{NLO}} = \int_n \mathrm{d}\tilde{\Phi}_n^{(4)}\,\mathcal{B} \quad + \quad \alpha_\mathrm{s} \int_{n+1} \mathrm{d}\tilde{\Phi}_{n+1}^{(4)} \left[\mathcal{R} - \mathcal{B} \otimes \mathcal{S}\right] \\ + \quad \alpha_\mathrm{s} \int_n \mathrm{d}\tilde{\Phi}_n^{(D)} \left[\tilde{\mathcal{V}} + \mathcal{B} \otimes \int_1 \mathrm{d}\Phi_1^{(D)} \mathcal{S}\right] ,$$

Many NLO ME calculators, but only a few automated ones. aMC@NLO and Sherpa fully automated; POWHEG-BOX is a framework to assist manual implementation.

Virtual terms from dedicated calculators, e.g. BlackHat/OpenLoops/NJETS/GoSAM via BLHA interface. Technically solved: processes like $W + 5$ jets or fully decayed $t\bar{t}$ and single-top are possible at NLO… *if you can spare the integration time!*

Biased event generation and weights

- For physics purposes, we want a flat distribution of event statistics across observables
- But many distributions fall fast: if we wait for an unbiased generator to produce a TeV-scale jet, we need to make as many events as the LHC does! *At sim-reco level…*
- Neat trick: bias the sampling to produce events not from a physical distribution but from a modified one, e.g. $\hat{p}_T^4 \cdot \hat{\sigma}(\Phi)$
- Experiments usually (also) create piece-wise “sliced” samples with matched min and max cuts on $2 \to 2$ subprocess $\hat{p}_T$



Distributions like this are hard to make without biasing

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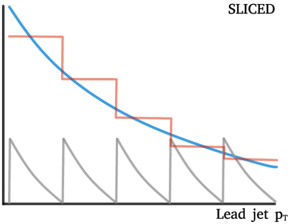
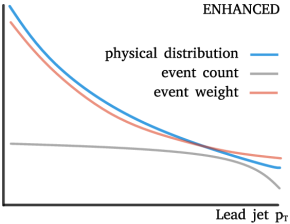
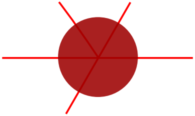




Parton showers

SHG step-by-step



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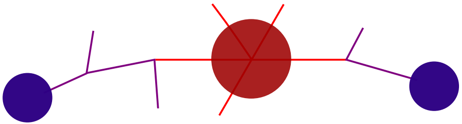

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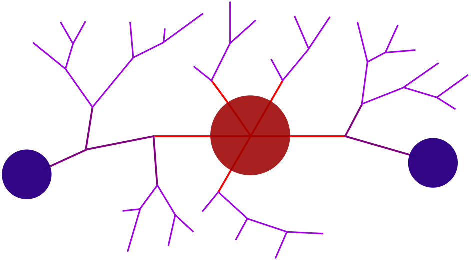


Splitting functions and resummation

Some parton–jet or parton–hadron duality: can compare *fixed-order partonic events* to data for IR-safe observables.

Soft and collinear phase-space, $1\,\mathrm{GeV} < p_\mathrm{T} \lesssim 20\,\mathrm{GeV}$, gets large *resummation corrections* from multiple QCD emissions.

Analytic resummation is process-specific and mathematically dense, especially beyond leading-log. But factorizes in the collinear limit: cross-section for process σ_0 with parton i to be accompanied by a collinear parton j with momentum fraction z:

$$\mathrm{d}\sigma \approx \sigma_0 \sum_{\mathrm{partons},i} \frac{\alpha_\mathrm{s}}{2\pi} \frac{\mathrm{d}\theta^2}{\theta^2} \,\mathrm{d}z\, P_{ji}(z,\phi)\mathrm{d}\phi$$

where θ is the angle between i and j and

$$\begin{aligned} P_{qq}(z) &= C_F \tfrac{1+z^2}{1-z}, & P_{gq}(z) &= C_F \tfrac{1+(1-z)^2}{z}, \\ P_{gg}(z) &= C_A \tfrac{z^4+1+(1-z)^4}{z(1-z)}, & P_{qg}(z) &= T_R(z^2+(1-z)^2) \end{aligned}$$

These are the spin-averaged QCD collinear *splitting functions* – or *DGLAP kernels*. Note divergences as $\theta, z \to 0$: dominates emissions.

Parton showers

Parton showers are Markov chain algorithms based on the QCD splitting functions → process-independent, approximate resummation. Creates parton multiplicities ∼ real-event hadron multiplicities

From splitting functions can calculate *probability of no emission* between scales Q and q (setting an IR cutoff for resolvability & perturbativity):

$$\Delta_i(Q^2, q^2) = \exp\left\{ -\sum_j \int_{q^2}^{Q^2} \frac{\mathrm{d}k^2}{k^2} \frac{\alpha_\mathrm{s}}{2\pi} \int_{q^2/k^2}^{1-q^2/k^2} \mathrm{d}z \, P_{ji}(z) \right\}$$

The famous *Sudakov form factor*. Can be inverted to generate a random parton emission with physical k distribution from a random number

Split into *initial-state* (ISR) and *final-state* (FSR) showers in SHGs:

1. ISR: generate high-p_T extra emissions on the incoming parton legs back to the proton (using *backward evolution*);
2. FSR: dress all final-state partons with a forward evolution down to the QCD perturbative cutoff Λ_QCD

More about showers

- In practice a more complex form is used, with running α_s (and carefully chosen running scale), spin effects, quark masses, etc.
- Any evolution variable $k^2 \propto \theta^2$ is permitted in the collinear limit and will resum the divergence.
  - But some are better than others: colour coherence (cf. Chudakov effect) effects suppress emissions outside the previous emission cone.
  - Quantum effect reproduced by θ-ordering and p_T-ordering, but not virtuality. All modern generators enforce colour coherence.

More about showers

- Initial state shower adds complication
  - Emissions modifying initial partons need to change the PDF x and flavour used ⇒ ISR Sudakovs include a PDF ratio term $\frac{x/z f_j(x/z, k^2)}{x f_i(x, k^2)}$ to ∼cancel up the chain
  - Forward-evolving from the hadron to find a consistent hard process configuration would be hopelessly inefficient ⇒ backward evolution.

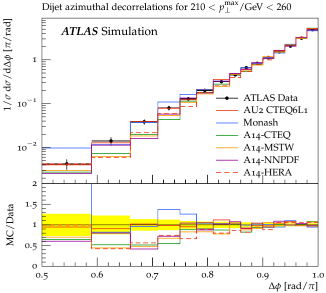
- Actually, $1 \to 2$ showers have problems:
  - Can't have finite relative p_T and real, on-shell partons since violates Lorentz symmetry ⇒ *reshuffling*
  - Much modern activity uses $2 \to 3$ dipole showers and higher variants – also for NLO subtraction compatibility: CSS, MatchBox, DIRE, Vincia, …

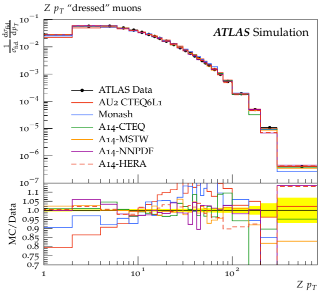
Forward evolution of spacelike shower, but more fun

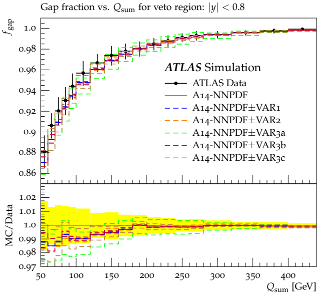
Shower observables

ISR: extra jets, jet distributions, $Z\ p_T$, gaps

NB. distinctly not collinear!





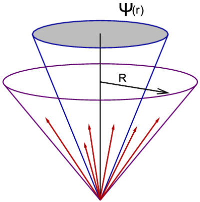


Shower observables

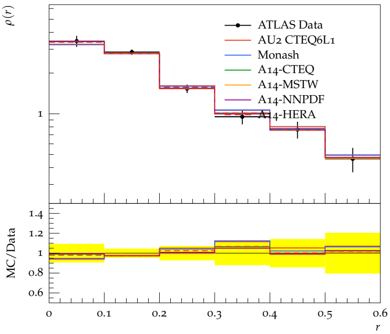
FSR: jet shapes, jet masses

i.e. adding structure to the parton = jet duality

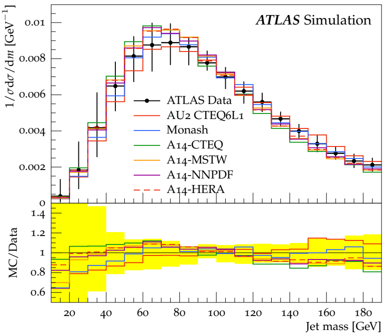
As jet scale increases, jets become increasingly collimated



Jet shape ρ for $p_\perp \in$ 30–40 GeV, $y \in$ 0.0–0.3



Cambridge-Aachen jets, $R = 1.2$, 300 GeV $< p_\perp <$ 400 GeV



ME–shower interfacing: "matching"

***Really* not enough space to do this topic justice: huge developments in last 20 years**

Issues are almost always because of double counting when the shower is used: an n-leg ME with parton shower *contains* the $n+1, \ldots$ terms.

To improve on the Born+shower approximation, need to **remove overlap.**

For LO multi-leg: MLM and CKKW schemes both designed to replace the shower's collinear splitting functions with proper matrix elements in the relevant (hard) phase-space

Phase-space slicing definitions took 10 years to iterate to better control. Introduces *merging scales*, which need to be chosen to minimise observable sensitivity: not "fire and forget" generation

Matching at NLO

Natural to go beyond tree-level matching: completely consistent NLO includes the Born, one-loop, and one-real emission amplitudes and all their interferences, *and* smoothly matches the real emissions between shower and ME.

Main benefit: NLO *scale stability*. Normalisation could always be taken from partonic highest-tech integrators, but (1-emission) shapes now also stable without disrupting formal accuracy of parton shower
⇒ rough rule of thumb: shapes from real, normalisation from virtual

- Addressed first by MC@NLO: extension of fixed-order subtraction to use shower-specific splitting functions: process-specific, $\sim 10\%$ negative weights.
- POWHEG[1] method later: "NLO matrix element correction". Closer to all-positive weights, and shower-independent. Convenience ⇒ large uptake.

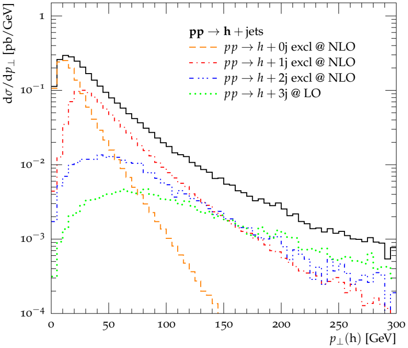
---

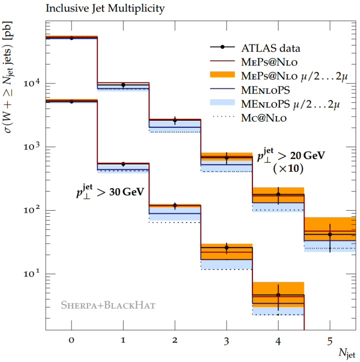
[1] Not, not, *not* 'PowHeg'!!! 'PoWHEG', if you must.

State of the art: NLO matching + merging

Now very impressive situation: automatic generation & merging of many NLO and LO multi-leg + shower in MEPS@NLO (Sherpa) and FxFx (MG5-aMC@NLO)

Bookkeeping *tour de force!* And at huge CPU cost in *unweighting*

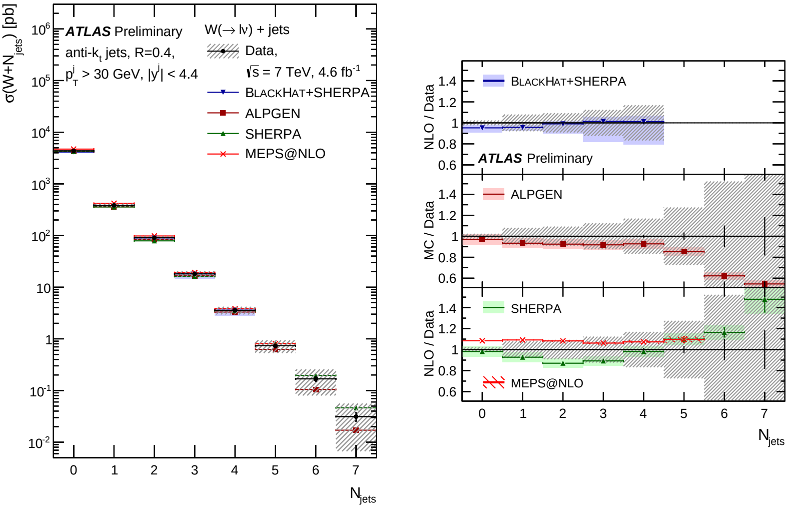




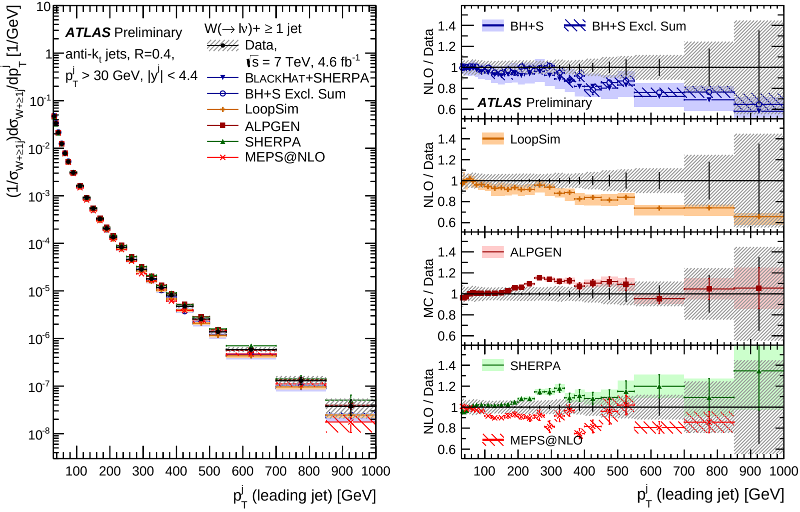
Increasingly NLO with EW corrections. NNLO-PS sometimes possible.

Which features are worth the CPU/opportunity cost?

Higher-order observables



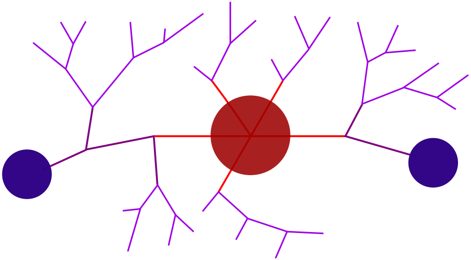
Higher-order observables



Non-perturbative stuff

(that we wish wasn’t there…)

SHG step-by-step



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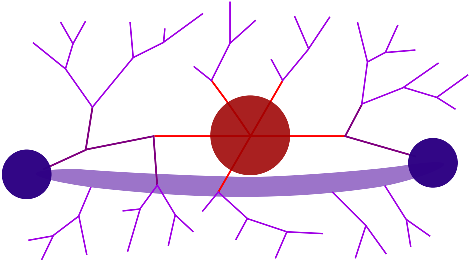

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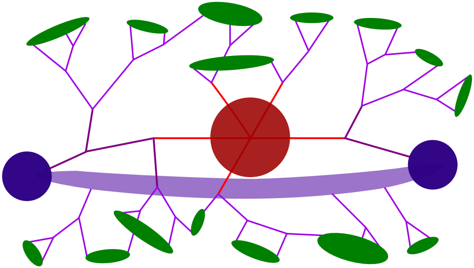

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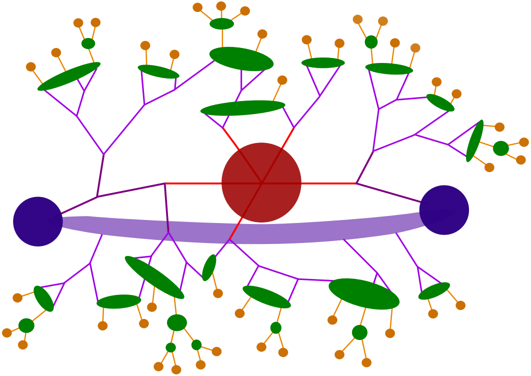
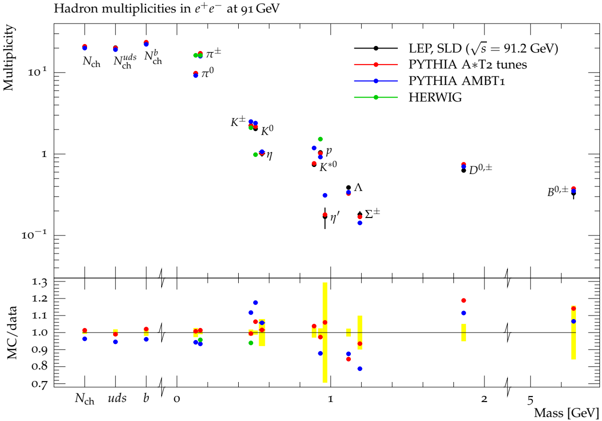


Hadronisation

- At scales below shower cutoff $Q_0 \sim \mathcal{O}(\Lambda_{\mathrm{QCD}})$, confinement means that physics is non-perturbative. **Source of most tuning params**
- Observe limited transverse momenta and Q^2-independent energy fractions: most quantum number flow done by the shower fragmentation, so hadronisation can be ~localised
- Two main modern hadronisation models: *Lund string and cluster*

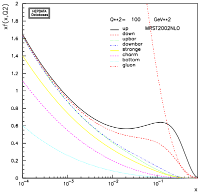


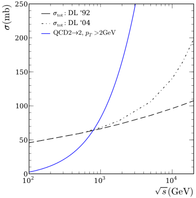
Hadronisation models

- **Lund string (Pythia):**
  - Inspired by *linear scaling of QCD potential* at large distances
  - Break colour strings to produce new quark pairs; gluons form kinks in strings
  - Lorentz invariance and LR-symmetry give Lorentz invariant *Lund symm frag function*
  - Kinematics well-described, but flavour – esp. baryons – not natural
- **Cluster hadronisation (Herwig, Sherpa):**
  - *Colour preconfinement*, seen in colour-connected neighbour parton mass spectrum
  - Non-pert $\rightarrow q\bar{q}$, then cluster colour singlets: requires finite gluon *constituent mass*
  - Clusters treated as *meson resonances*
- Both models (except Sherpa) also contain *colour reconnection* heuristics
- **Tuning!**

Underlying event

HERA data show inclusive jet cross-section rising strongly with energy due to low-x PDFs (esp. gluon)
$\Rightarrow$ unitarity violation

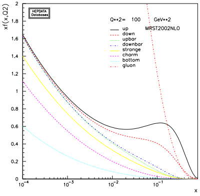


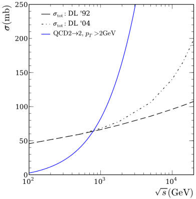


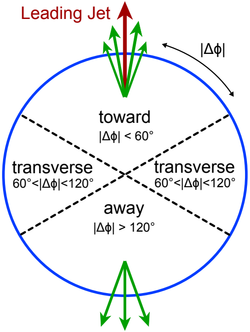
- Eikonal models interpret the bottom-up to top-down σ ratio as mean number of *multiple-parton interactions (MPI)* $\Rightarrow$ sample Poisson to make n pQCD subprocesses
- Hadron impact parameter $\sim 1/Q \Rightarrow$ transverse overlap also important
- Low hard-process scale $Q \Rightarrow$ low overlap & low n: "minimum bias" cf. pile-up
- High hard-process scale $Q \Rightarrow$ total overlap & high n: *pedestal effect* → "underlying event"
- Extra details: $\hat{p}_T$ cutoff/screening, proton overlap form factor, colour reconnection. **Tuning!**

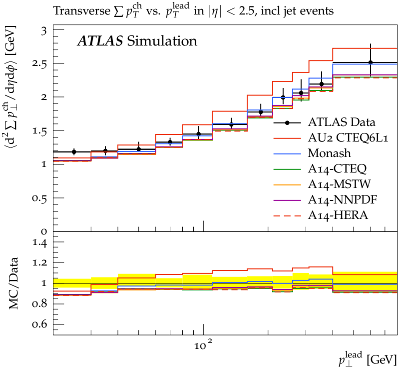
Underlying event

HERA data show inclusive jet cross-section rising strongly with energy due to low-x PDFs (esp. gluon)
$\Rightarrow$ unitarity violation



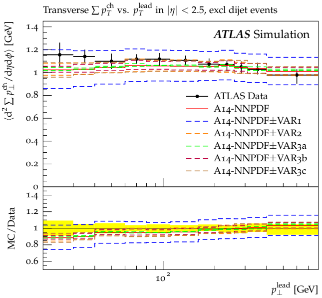






MC tuning

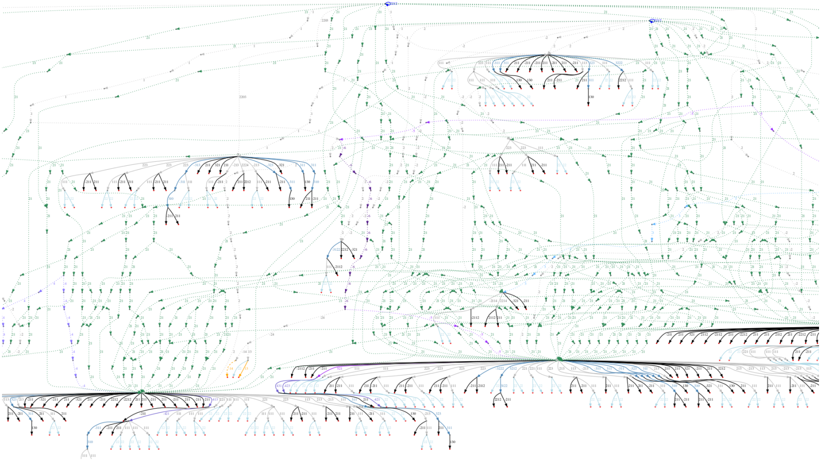
- Freedom to describe data with generator models, via the *ad hoc* and beyond-fixed-order components: MPI, hadronisation, $\sim$ showers
- Need to be careful! A pragmatic trick at LO may backfire spectacularly when a better ME is added. Knowing the *limits* of a generator configuration is important
- A global view is crucial: one number/distribution can always be overtuned at cost of others
- Rivet & Professor/Apprentice tools used to build tunes & *eigentunes*



Using MC events…wisely

Example SHG event

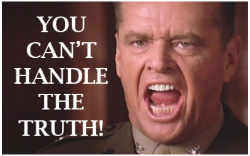
(Part of) a single-top HepMC event graph:

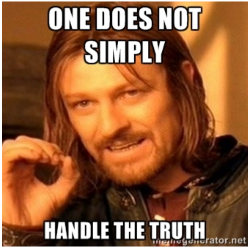


Ouch! How to safely *use* this??

Caveats on event record interpretation

- **The SHG generator (or LHE) event record is often called “truth” – a dangerous phrase.**
- We’re doing quantum mechanics: there is no unambiguous truth!
  ⇒ event records are half-physics, half-debug-info…and zero indication of amplitude interference
- It gets worse: kinematic frames aren’t defined (until the final-state) & momentum isn’t necessarily conserved at vertices!
- **BEWARE!!**





Caveats on event record interpretation

- That said, like all good myths, there is a core of truth to the widespread physical interpretation of event records
- And sometimes precision EW or PDF theorists will request correction to partonic level rather than forward-folding of their calculations, e.g. "Born-level Z".

  NB. expts don't have to say "yes"!
- First **think about the physics** – e.g. is there a real distinction between hard photons and shower photons? Good discipline/introspection anyway!
- And first try to do what you need directly from the physical hadrons etc. See Rivet ↗ & ATLAS PUB note on safe truth observables ↗

Apply brain!

Conclusions

Summary

- Event generators are super-, super-important for LHC physics
- And demands are only increasing: we demand processes and levels of data description (and predictivity) that would have been laughed at 10 years ago
- Both experiment and theory owe a great deal to the few phenomenologists who've provided us with these codes
- SHGs based on a core of perturbative QCD (& EW) of increasing sophistication. And increasing CPU cost…
- Wrapped with perturbative iterated parton showers ⇒ resum logs & generate a good approximation to "real" final-states. Plus pheno models for the stuff we don't understand *ab initio*
- **Follow-up material:**
  MCnet review – arXiv:1101.2599
  Hoeche review – arXiv:1411.4085
  "Practical Collider Physics" – AB, White, White
  "QCD & Collider Physics" – Ellis, Stirling, Webber
  "QCD" – Dissertori, Knowles, Schmelling
  MCnet summer schools: 2018 2019 2022

Some hands-on exercises

Being able to run event generators yourself (rather than just using experiment samples) is a big advantage.

- Get Pythia 8 and generate QCD dijet events with ME $\hat{p}_T$ cutoff of 50 GeV. Analyse with Rivet's `MC_JETS` analysis. What does it look like if you change the cutoff? How about the shower α_s?
- Get the POWHEG-BOX heavy-flavour (hvq) process and generate $t\bar{t}$ events. Shower with Pythia and compare to top-pair production in LO Pythia using also the `MC_TTBAR` analysis: differences in normalisation? shapes?
- Get MG5 and generate a `p p > z > mu+ mu-` process with Pythia showering. Use `add process` to merge this with $+1, 2$ jets MEs. Analyse with Rivet or MadAnalysis5. What changes?
- Generate a BSM process, e.g. SUSY gluino pair production in Pythia's built-in processes (you will need an SLHA file, e.g. from an experiment publication), or a FeynRules UFO model like SMEFTsim ↗ in MG5

The MCnet hepstore ↗ Docker images may be useful