Event generators in LHC Run 2

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Introduction

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"Monte Carlo" is ubiquitous in LHC experimental work. Contrast to \sim 1980 when experimentalists wrote their own...

- But event generators are often treated as *black boxes...* which is rarely a good idea! A little extra understanding can go a long way.
- This talk is a mix of ~pedagogical review of standard event generator principles, and unvarnished personal opinion.
- Time forces me to be superficial!
 Watch for analogies and waving hands...
- If you're going to know one "extra" bit of theory, then the principles of event generation is a good choice.

Introduction

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Early excuse: I'm an experimentalist, i.e. much more a user than developer. Much of modern MC's devil is in the detail... and only discovered by writing one. **Apologies in advance to the experts!**

What is an event generator?

- The phrase "event generator" is rather overloaded: many pheno people refer to partonic MC integrators (e.g. MCFM, TOP++, NLOJET++, ...) as event generators
- ▶ 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
 - Historically they were also *unweighted* a few words on this later
- Integrators still very important as a source of the most high-tech cross-section normalisations etc. – but I won't discuss them
- 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 quantum field theory
 - but *approximately* since we can't calculate all-orders, full-multiplicity processes explicitly
- Since QCD is the strongest force, QCD effects usually dominate MC implementation

Shower & hadronisation event generators (SHGs)

Okay, so 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; helping the above ⇒ papers, careers, hero worship...



A selective list

Partonic subprocess generators (used as SHG input via LHE):

- Multi-leg LO: MadGraph, AlpGen, (Sherpa)
- NLO (+ multileg): POWHEG-BOX, (MadGraph5-)aMC@NLO, (Sherpa), MINLO
- Specialist processes: WHiZard, Protos, HEJ; Charybdis2, QBH, BlackMax, ...

Main general purpose event gens:

- FORTRAN: FHerwig and FPythia
- C++: Sherpa, Herwig++/7, Pythia 8
- You may be excited about BSM, but most of the MC effort is on boring old QCD

Afterburners:

• EvtGen, Photos, Tauola, Jimmy

Specialist all-in-one:

- Min bias & air showers: PHOJET, EPOS, QGSJET, SYBILL
- Heavy ion: HIJING, HYDJET, Starlight
- Sherpa is sort-of a general-purpose all-in-one

Experiment data processing chain

Typical experimental use of generators is to feed their output (as HepMC or LHE files/objects) into detector sim based on Geant 4.

Then apply the same reconstruction algs 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 a SHG



ME Shower Hadronisation Decays ISRUEPDFsBSM, $diffraction, \tau,$ $\gamma, B...$

This diag ignores UE and ISR

Anatomy of a SHG

Or, alternatively...



Anatomy of a SHG

Or...



Matrix elements





Matrix elements

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

$$\begin{split} \sigma &= \sum_{a,b} \int_{0}^{1} \mathrm{d} x_{a} \mathrm{d} x_{b} \int f_{a}^{h_{1}}(x_{a},\mu_{F}) f_{b}^{h_{2}}(x_{b},\mu_{F}) \, \mathrm{d} \hat{\sigma}_{ab \to n}(\mu_{F},\mu_{R}) \\ &= \sum_{a,b} \int_{0}^{1} \mathrm{d} x_{a} \mathrm{d} x_{b} \int \mathrm{d} \Phi_{n} f_{a}^{h_{1}}(x_{a},\mu_{F}) f_{b}^{h_{2}}(x_{b},\mu_{F}) \\ &\times \frac{1}{2\hat{s}} |\mathcal{M}_{ab \to n}|^{2}(\Phi_{n};\mu_{F},\mu_{R}) \,, \end{split}$$

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

Squared amplitude may be computed from Feynman diagrams directly, a bit more efficiently via helicity amplitudes, or via twistor/unitarity methods like Berends-Giele, MHV, OPP, BCFW, ...

The "MC" comes in because the integral is done by Monte Carlo sampling. In 4(n - 1) phase space dimensions, with a strongly diverging matrix element, this is not a trivial undertaking!

Sampling

An extraordinary number of problems can be solved by MC sampling!

MC wins when number of dimensions becomes large – error always reduces as $\sqrt{\text{samples}}$, rather than degrading with dims.

Naïve sampling doesn't get far: easy to spend all CPU/disk space generating *atypical points* which which are dwarfed by a lucky strike on the typical set.

A better strategy:

- Jacobian-transform phase space to remove divergent structures;
- ► But there are many characteristic divergences in matrix elements ⇒ multi-channel integration
- Choose an (over)estimator which can be sampled efficiently for each channel e.g. via inverse transform
- Use a standard MC sampling method e.g. Metropolis and combine channels
- More refinement: adaptive sampling algorithms to "learn the space"

Matrix element generators

- Historically, Herwig and Pythia contained large libs of lowest-order MEs
 - Not scaleable! C++ Herwig and Pythia ME libraries are much smaller ⇒ LHE input
- New industry in automatic partonic event generators
 - Alpgen, MadGraph and Sherpa were first to generate multi-leg-LO *Feynman-based MEs and sample events automatically*
 - Sherpa's newer COMIX ME generator uses Berends–Giele recursion: faster & better convergence
 - Sherpa 2, aMC@NLO (and POWHEG-BOX) now generate NLO (1-loop) events automatically with a little help
 - BSM: define new physics model at Lagrangian level via FeynRules. *Feed to ME generator*, e.g. MadGraph, Sherpa, ... via UFO files to make events in arbitrary models!
- Integration time can take weeks for complex processes!! Parallel processing needed.

(Far) beyond LO

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

Extra partonic emissions at tree-level increase the final state multiplicity and change the event kinematics directly. Calculation is automated in Alpgen, MadGraph & Sherpa, via Feynman diagrams / BG recursion / etc. and multichannel integration.

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 S which encodes real emission divergence structure so $\mathcal{R} - \mathcal{B} \otimes S$ is finite:

$$\begin{split} \sigma^{\rm NLO} &= \int\limits_{n} d\tilde{\Phi}_{n}^{(4)} \mathcal{B} + \alpha_{\rm s} \int\limits_{n+1} d\tilde{\Phi}_{n+1}^{(4)} \left[\mathcal{R} - \mathcal{B} \otimes \mathcal{S} \right] \\ &+ \alpha_{\rm s} \int\limits_{n} d\tilde{\Phi}_{n}^{(D)} \left[\tilde{\mathcal{V}} + \mathcal{B} \otimes \int\limits_{1} d\Phi_{1}^{(D)} \mathcal{S} \right] \,, \end{split}$$

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...*if you can spare the integration time!*

Both LO multi-leg and NLO become even more complicated when parton showers are involved...

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!
- Neat trick: bias the sampling to produce events not from a physical distribution but from a modified one, e.g. p⁴_T σ(Φ)
 - This feature missing from MadGraph so far: *a project for someone!*



Distributions like this are hard to make without biasing

Biased event generation and weights

- Experiments usually create piece-wise "sliced" samples with matched min and max cuts on $2 \rightarrow 2$ subprocess \hat{p}_T
 - Note that p̂_T isn't well-defined for higher final-state multiplicities – but similar quantities can be defined
 - p̂_T slices still contain falling distributions within slices – can be *post hoc* flattened cf. ATLAS "JZ"
 - Maybe this will change, since weights have become more normal
- Weight *stability* is still important biasing is observable-specific



Distributions like this are hard to make without biasing

Parton showers





Parton showers and resummation

Limited parton-jet/parton-hadron duality allows us to compare IR-safe observables to data But even these must account for higher order contributions from enhanced regions of phase space: soft and collinear.

Resummation (why the *re*-?) sums effects of gluon emissions in these regions.

Parton showers are Markov chain algorithms based on the collinear limit of QCD splitting, formulated for process independence. As well as performing an approximate resummation, they generate parton multiplicities compatible with hadron multiplicities (via hadronisation and decays).

Split into timelike "FSR" and spacelike "ISR" showers in SHGs.

PS formalism – splitting functions

Cross-section for process σ_0 with parton *i* to be accompanied by a collinear parton *j* with mom 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

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

These are the spin-averaged QCD collinear *splitting functions* – or *DGLAP kernels*

PS formalism – Sudakov form factor & MC

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

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

This is the famous *Sudakov form factor*. Describes QCD emissions cf. a non-linear radioactive decay, where individual decay rate depends on the time.

In MC, choose a random number $\mathcal{R} \in [0, 1]$, and solve $\Delta_i(Q^2, q^2) = \mathcal{R}$ to create an emission of parton *j* and scale *q*. Then choose *z* from the splitting function.

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 k² ∝ θ² 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

 - Forward-evolving from the hadron to find a consistent hard process configuration would be hopelessly inefficient ⇒ backward evolution.
- Actually, $1 \rightarrow 2$ showers have problems:
 - Can't have finite relative *p*_T and real, on-shell partons since violates Lorentz symmetry ⇒ *reshuffling*
 - Much modern action is with 2 → 3 dipole showers and higher variants – also for NLO subtraction compatibility: CSS, MatchBox, 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





ME-ME & ME-shower mixing





ME–shower interfacing: LO

Really not enough space to do this topic justice: huge developments in last 10 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, ... 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 collinear shower 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

ME-shower interfacing: NLO

Parallel problem of improving on Born LO + shower with a single 1-loop NLO matrix element addressed first in MC@NLO

Extension of subtraction to use shower-specific splitting functions \Rightarrow works, with $\sim 10\%$ negative weights. And required per-process, per-SHG implementation: uptake only in special areas

POWHEG method came later: "NLO matrix element correction". Closer to all-positive weights, and shower-independent. Convenience \Rightarrow large uptake.

- Details of shower interface not 100% clear: formally beyond-NLO effect, but can be large
- Truncated/vetoed showers & mismatches of ordering variable
- Evolution: MINLO scheme, HDAMP etc. freedom in separating/transitioning from hard to soft phase space

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

ME-shower interfacing: NLO matching + merging

Now very impressive situation: automatic generation & merging of many NLO and LO multi-leg + shower in MEPS@NLO (Sherpa) and FxFx (MG-aMC@NLO)! At parton-level cf. BlackHat+Sherpa

Virtual terms from dedicated integrators e.g. BlackHat, OpenLoops, ... via BLHA format. Bookkeeping *tour de force!*



Higher-order observables



Higher-order observables



Non-perturbative stuff (that we wish wasn't there...)









Hadronisation

- At scales below shower cutoff Q₀ ~ O(Λ_{QCD}), confinement means that physics is non-perturbative. Source of most tuning params
- ► Observe limited transverse momenta and Q²-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 is arguably the most successful hadronisation model, used in Pythia

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 $g \rightarrow q\bar{q}$, then cluster colour singlets: requires finite gluon *constituent mass*
 - Clusters treated as *meson resonances*
- Both models (except Sherpa) also contain *colour reconnection* heuristics

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 multi-parton interactions – sample Poisson dbn to make n "hard" subprocesses.
- ► Hadron impact parameter $\sim 1/Q \Rightarrow$ transverse overlap also important
- ► Low hard-process scale Q ⇒ low overlap & low n: "minimum bias" cf. pile-up
- ► High hard-process scale Q ⇒ total overlap & high n: "underlying event"
- Extra details: p_T cutoff/screening, proton overlap form factor, colour reconnection. Tuning!

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NB: multi-leg shower is key

MC tuning

- Freedom to describe data with generator models, via the *ad hoc* and beyond-fixed-order components: MPI, hadronisation, ~ 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 (tutorial!) & Professor ⇒ tunes & eigentunes: estimate residual systematic uncertainties beyond scale & PDF variations. But much more work to evaluate: no option for reweighting





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Conclusions

Example SHG event

$t\bar{t}$ event graph:



Plots by mcview/mcdot

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 fragmentation photons? Good discpline/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!



Summary

- Event generators are super-, super-important for LHC physics
- And demands are only increasing: we demand processes and levels of data description (and extrapolation 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...even when they go wrong!
- SHGs are based on a core of perturbative QCD (& EW...) at increasingly sophisticated order.
- ► Wrapped with perturbative iterated parton showers ⇒ resum logs & generate a good approximation to the high-multiplicity process we wanted. And pheno models for the stuff we don't understand *ab initio*
- Follow-up material: MCnet review arXiv:1101.2599; "QCD & Collider Physics" – Ellis, Stirling, Webber; "QCD" – Dissertori, Knowles, Schmelling; MCnet etc. summer schools

Opinions/speculation for Run 2

- New generation of tools firmly established: FeynRules, MadGraph-aMC@NLO, POWHEG, Sherpa, Pythia 8, Herwig++
 - Modularity, albeit not quite the way that was expected, cf. **ThePEG**. Instead: LHE format, FeynRules
 - FHerwig is dead; Alpgen and FPythia not dead yet...but close
- Showered NLO is the new normal, and showered multi-leg, multi-NLO is becoming normal
 - Present: SM processes at NLO in Sherpa / POWHEG-BOX, aMC@NLO + Pythia 8/Herwig++/7 for LO and NLO. FeynRules for general BSM.
 - Future?: MC@NNLO? CPU?! More shower developments: beyond leading colour, NLO splittings? ME improvements increasingly reduce dependence on shower, but resummation/matching effects aren't always small & improvement always welcome

 Trends set to continue: more demands of accuracy and more demanding processes

- Realise that the "NLO" brand is not everything: observables can still be LL, matching details/systematics not yet watertight
- ► Everything needs to work! No point in pQCD sturm & drang if the b-decays crap up! ⇒Big demands also on tuning & systematic validation systems