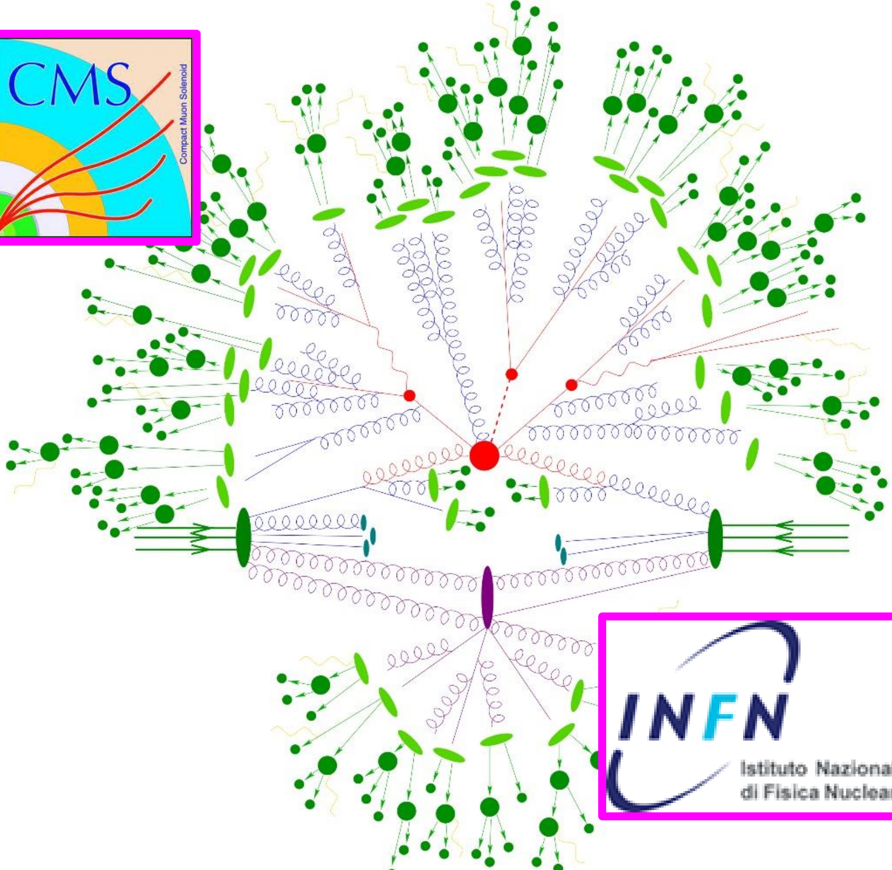
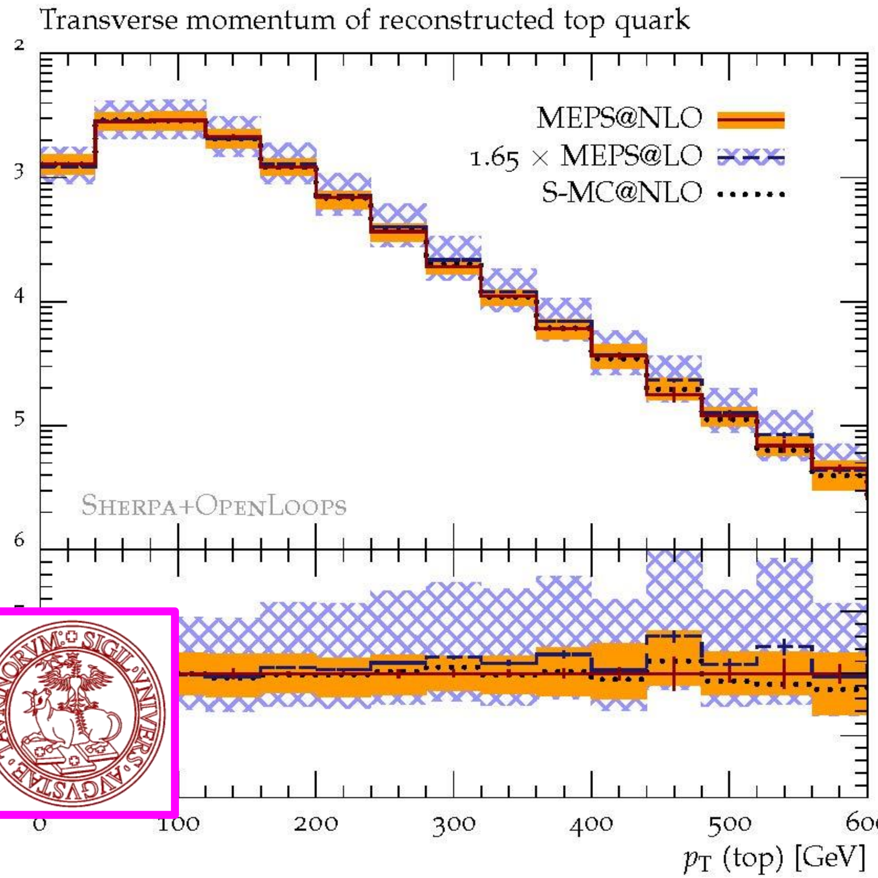




Use of Monte Carlo simulation at the LHC

Roberto Covarelli (*University / INFN of Torino*)

XIII meeting on B-Physics - Napoli, 23 May 2017

Outline

- MC tools widely used at the LHC
  - Matrix-element generators and parton showers
  - MC for B-physics
- Assessing theory uncertainties from MC
  - Matrix-element reweighting
  - Recent works on parton-shower uncertainties
  - PDFs and underlying-event tunes
- Technical aspects
  - General issues of large-sample generations
  - Issues specific to B-physics

Monte Carlo tools

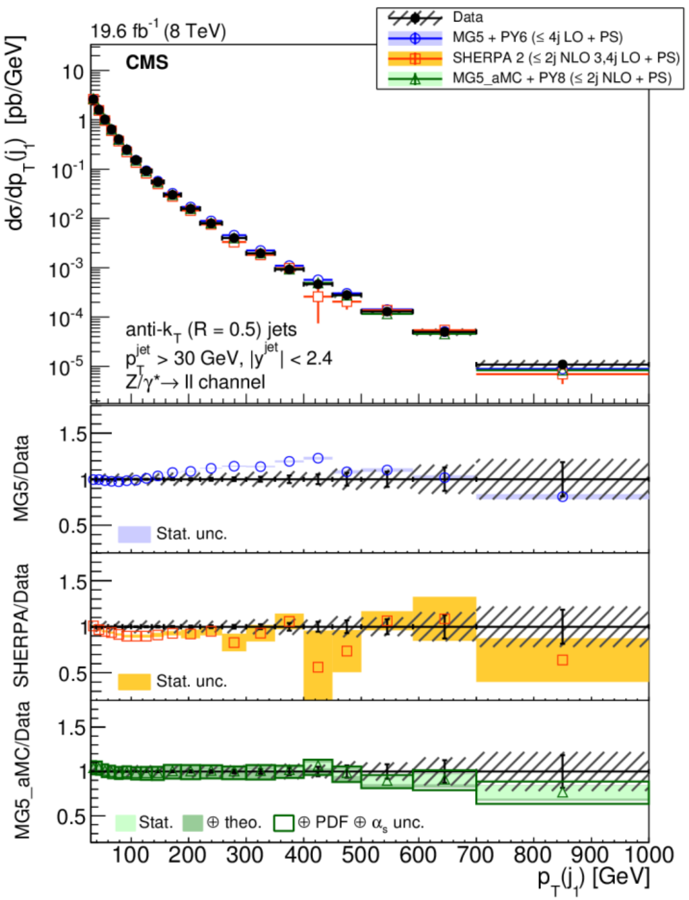
Use of MC in pp experiments

- 3 main ways of exploitation:
  1) Signal acceptance and efficiency: associated uncertainties are typically very small (cancellation in ratios). Severe mismodeling issues can happen only in case of large changes in kinematics, e.g.:
     - LO vs. NLO gg → H production
     - Simulation vs. missing simulation of g → b bbar … etc.
  2) Background estimation for rare signal searches. Should be mitigated where possible by use of data control samples (sidebands etc.) otherwise MC uncertainties enter in full
  3) Traning samples for multi-variate analyses (MVA): propagation of MC uncertainties / mismodeling not easy to assess, especially in case of non-analytical MVA (e.g. BDT)

MC generator categorization

- Order in QCD:
  - LO or NLO (first NNLO generators appearing in recent years just for specific processes, e.g. $gg \to H$)
- Purpose:
  - Full-event generators (e.g. Pythia8, Herwig7, SHERPA) or just for some stages of MC generation:
    - Matrix-element, i.e. up to parton-level (e.g. MadGraph5_aMCatNLO)
    - Parton showers
    - Applications for particle decays (e.g. EvtGen, Tauola)
  - Use of staged generation requires special treatment of physics effects («matching») and software interfacing
- Automation:
  - Can only simulate specific processes (e.g. POWHEG, Pythia8) or a generic $pp \to X$ process can be defined by user (e.g. SHERPA, MadGraph5_aMCatNLO)

Matrix-element generators

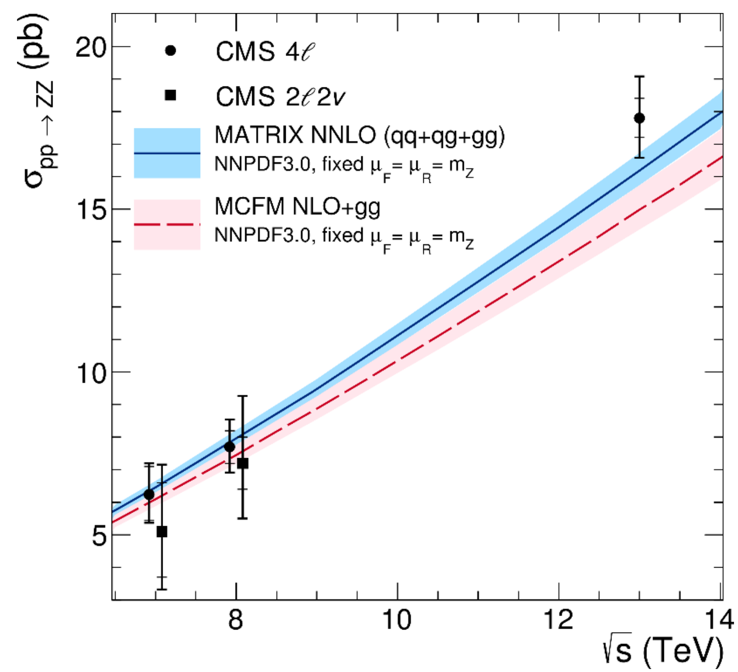


CMS-SMP-14-013, submitted to JHEP

- NLO QCD event generation is now the standard (SHERPA, POWHEG, MadGraph5_aMCatNLO)
- Specific cases where LO is still used:
  - Final states with large particle multiplicities (e.g.V + 4jets)
  - NP signals where NLO calculations are not available/implemented
  - Final states with particularly complicated kinematics (e.g. pp → G* with full tensor structure)
  - …etc.

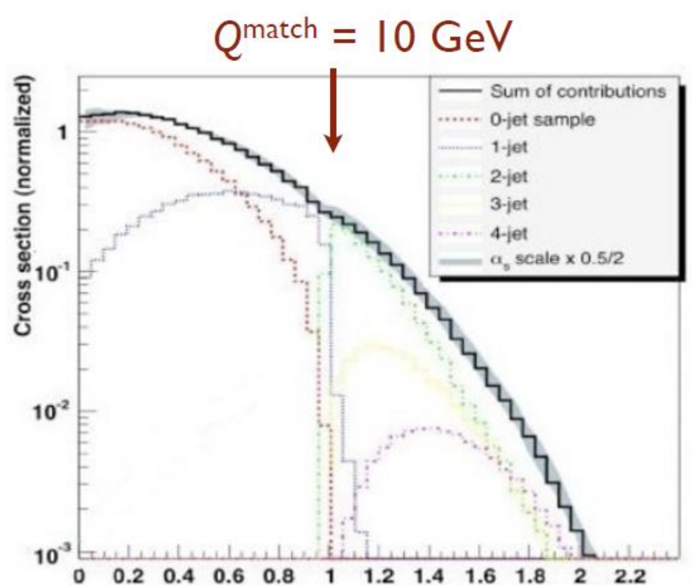
Higher-order QCD corrections

- NLO ensures:
  - Reasonable QCD scale uncertainties → o(10%) for V+jets / ttbar
  - Quite accurate description of kinematics when matched to a parton shower (NLO+PS), except for some rare processes (e.g. those with a box diagram at the lowest order)
- In some cases where higher-order calculations are needed, experiments use k-factors ($k = \sigma_{NNLO}/\sigma_{NLO}$)
  - Integrated, i.e. scale cross-section by a constant number
  - Differential vs. specific process variables (event «reweighting» when filling MC distributions)



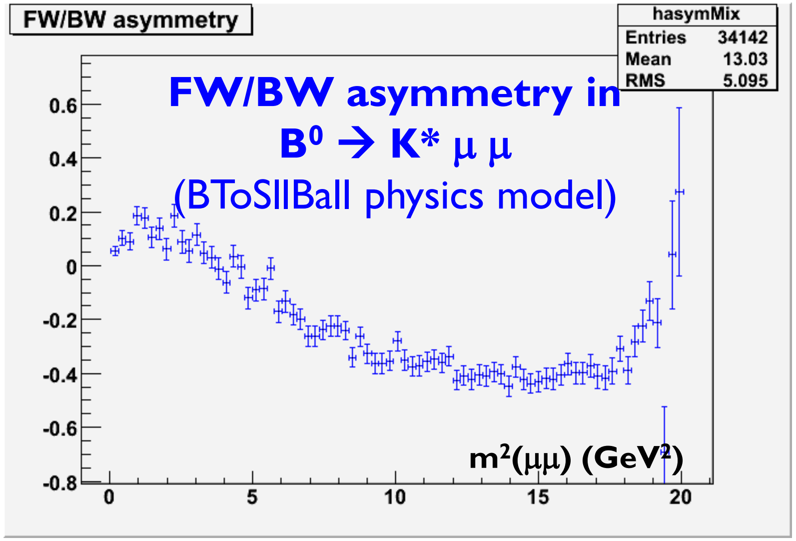
Parton showers

- Most matrix-element generators (basically all except SHERPA) need matching with an external parton shower to produce finalized pp events
- Pythia8 and Herwig++ (recently updated to Herwig7) are the two most widely used in LHC
- Matching is not a trivial task as it must deal with jet double counting:
  - An event with e.g. V+2jets can have two real g/q emissions from the ME, or one from ME and one from PS etc.
  - Theoretical recipes exist (MLM for LO, FxFx for aMCatNLO, emission veto for POWHEG etc.) and are included in PS tools



External decay programs

- PS tools provide their own particle decay utilities
  - For specific signals, external decay programs can be used
- EvtGen managing complex B (and hadron) decays
  - Created in BaBar, now maintained by the LHCb Warwick group
  - http://evtgen.warwick.ac.uk/
  - Spin amplitudes, CPV, automatic PHOTOS interface, etc.
- Interfacing to other tools is apparently trivial
  - Veto particle decays in other tools, if known to EvtGen
- In practice, many subtle issues
  - Coherence of PDG data in the two generators
  - Signal particles could be within an EvtGen decay tree
  - Fall-back to Pythia for high-multiplicity decays etc.

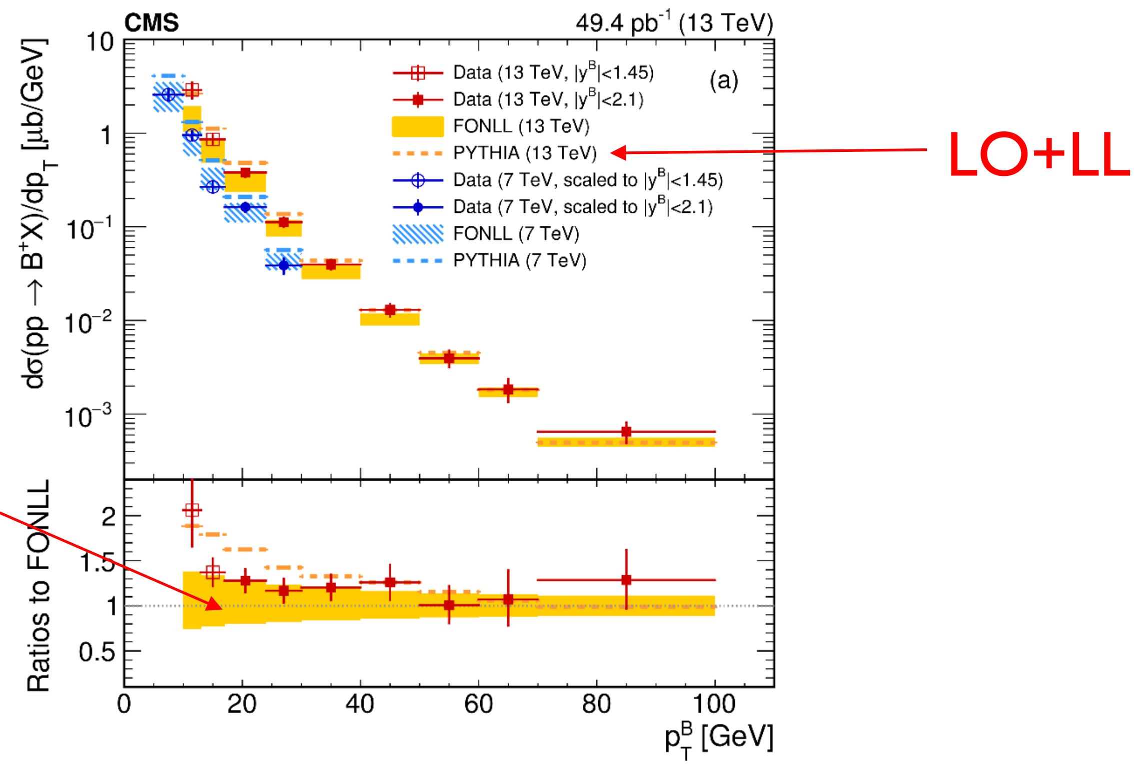


Use of MC in B-physics experiments

- 3 main ways of exploitation?
  1) Signal acceptance and efficiency: associated uncertainties are typically very small (cancellation in ratios). Severe mismodeling issues can happen only in case of large changes in kinematics
     - LO vs. NLO: really important?
  2) ~~Background estimation for rare signal searches. Should be mitigated where possible by use of data control samples (sidebands etc.) otherwise MC uncertainties enter in full~~

     ALMOST NEVER USED
  3) Traning samples for multi-variate analyses (MVA): propagation of MC uncertainties / mismodeling not easy to assess, especially in case of non-analytical MVA (e.g. BDT)

HQ production: Pythia8 vs. FONLL



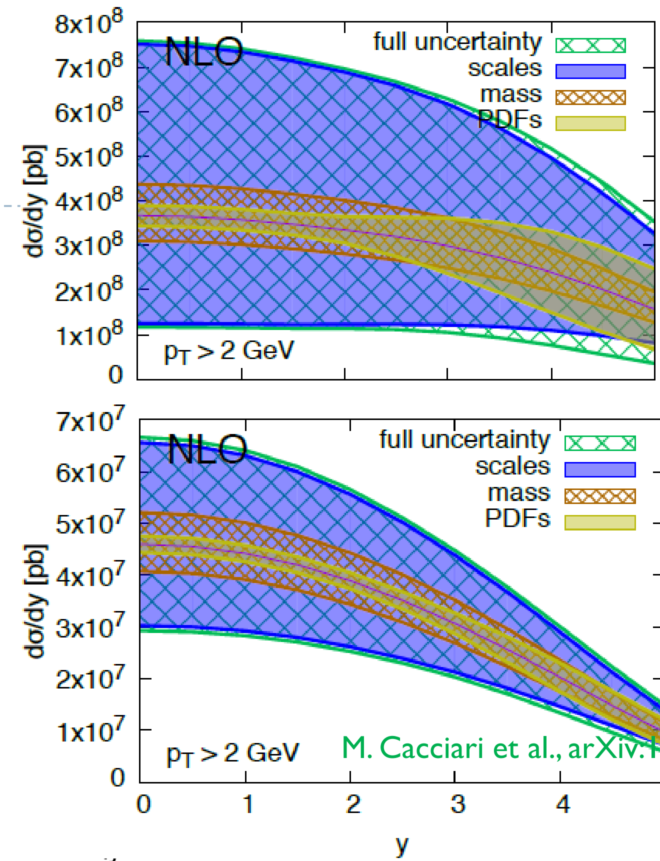
CMS-BPH-15-004, submitted to JHEP

- In many practical cases, LO sufficient for B production kinematics
  - Generation speed is more important, see next slides

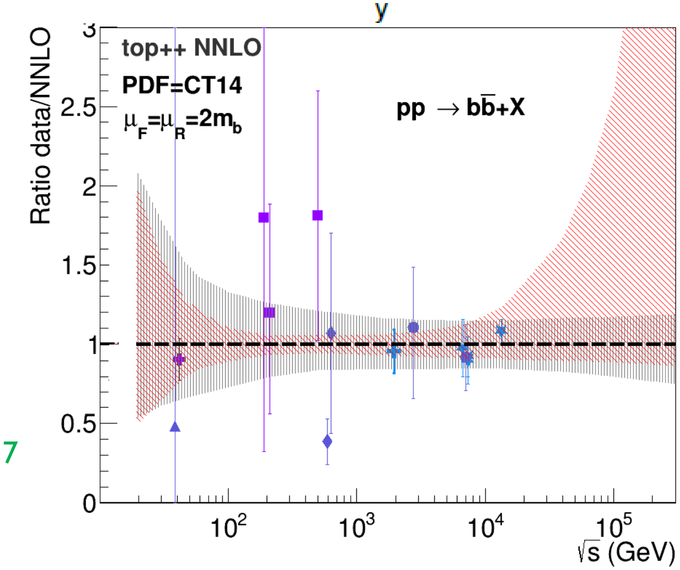
R. Covarelli

HQ production: beyond NLO?

- Scale uncertainties still not so small, especially for ccbar
  - Dominant vs. other sources (gluon PDFs, b and c mass)
- Ratios at different √s remove such uncertainties
- First attempts to use Top++ NNLO computator (Mitov and Czakon, 2013) applied to other quarks
  - Encouraging, but NNLL seems not possible yet (essential for low p_T production)



M. Cacciari et al., arXiv:1507.06197



D. D'Enterria, talk at Moriond 2017

Monte Carlo uncertainties

Reweighting

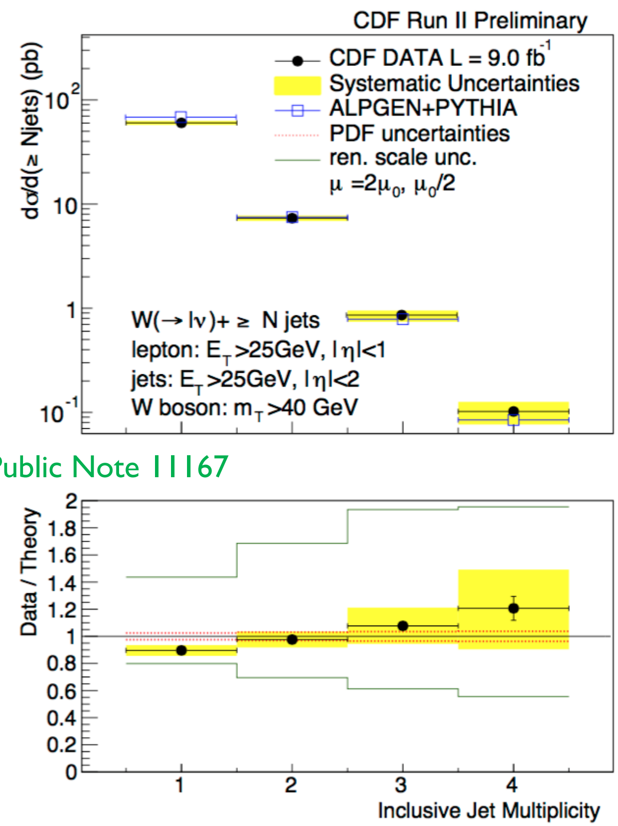
- Nowadays matrix-element generators can compute variations of certain calculation parameters on an event-by-event basis and write the result as a per-event weight
  - Most common
    - QCD renormalization and factorization scales (7 to 9 variations corresponding to x0.5, x2 in all possible combination
    - PDF variations (can be 100's of them)
  - Written in LHE files in standard form

```
<weightgroup combine="envelope" name="scale_variation">
<weight id="1001"> muR=1 muF=1 </weight>
<weight id="1002"> muR=1 muF=2 </weight>
<weight id="1003"> muR=1 muF=0.5 </weight>
```

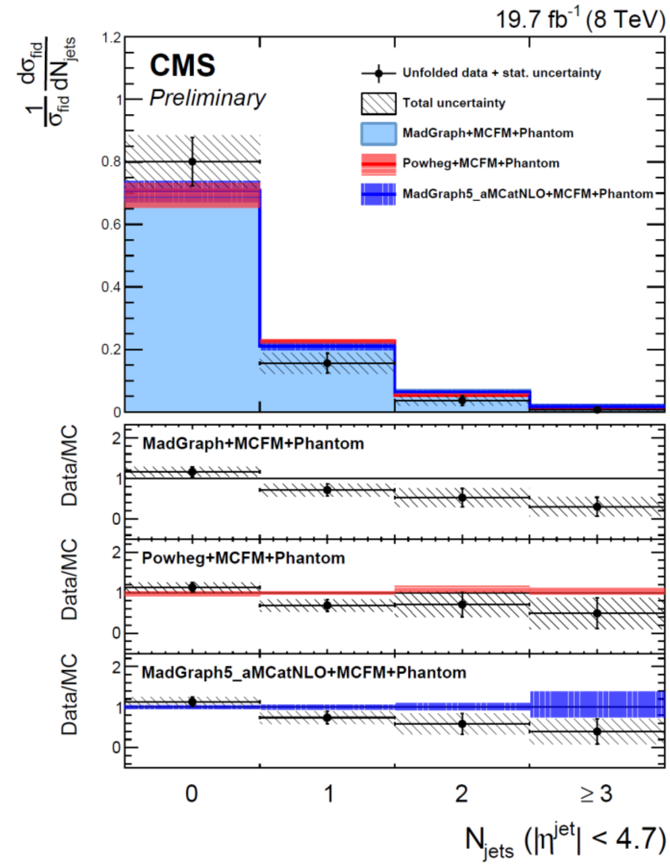
```
<weightgroup combine="hessian" name="PDF_variation">
<weight id="2001"> PDF set = 260001 </weight>
<weight id="2002"> PDF set = 260002 </weight>
<weight id="2003"> PDF set = 260003 </weight>
```

- Crucial for use in experiments!
  - Would be impossible to produce 100's of samples, one per variation

Is this the full theory uncertainty?



CDF Public Note 11167



CMS-PAS-SMP-15-012

- LO vs. NLO cannot be responsible for such a difference

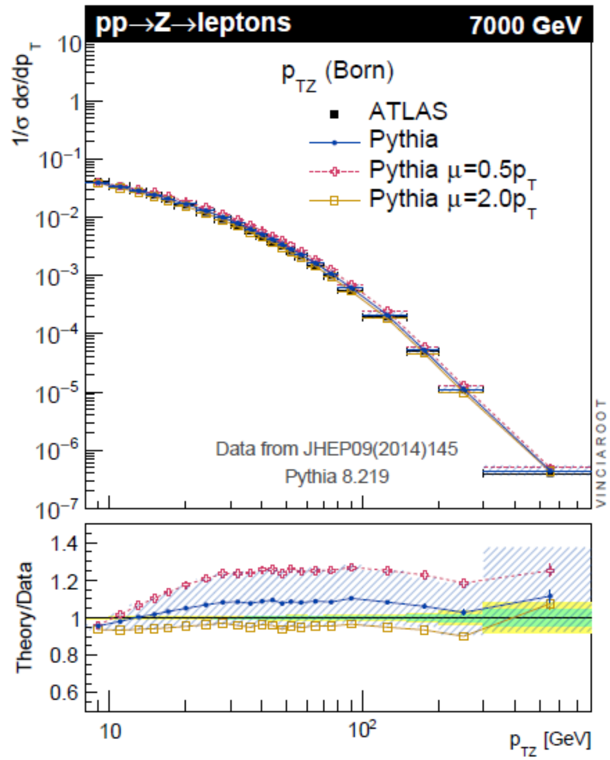
Parton shower uncertainties

- The matrix-element generator uncertainty is not the end of the story → parton shower uncertainties can be large
  - Especially important if MC used for background estimation
  - Even more if variables are heavily affected by showering/fragmentation/hadronization, e.g. jet substructure, q/g discrimination etc.
- Until 2016, mixed recipes used in experiments
  - Totally neglected
  - Used Pythia vs. Herwig difference in relevant variables
  - Used ME-consistent up and down μ_R variations
- In very recent years, substantial progress on the matter
  - Improved PSs (DIRE, VINCIA) EPJC 76 (2016) 589, arXiv:1705.00982
  - Three simultaneous works from authors of Pythia, Herwig and SHERPA clarifying the matter of PS uncertainties

arXiv:1605.01338, arXiv:1605.08352, arXiv:1606.08753

The Pythia8 example

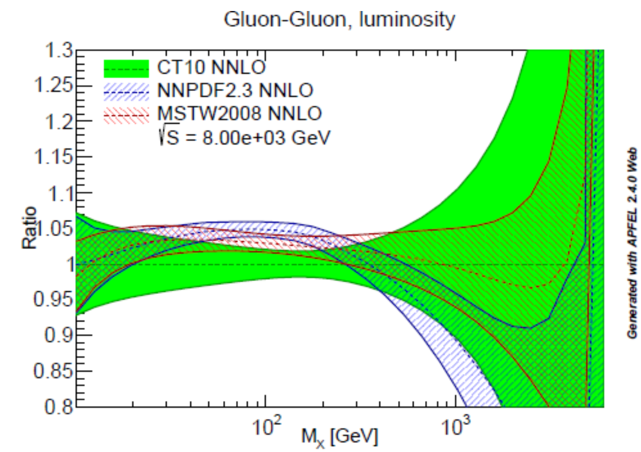
- More difficult to have per-event weights in PSs because of their literal «MC» nature (acceptance-rejection algorithms)
- In Pythia8 now available from a specific «recycling» of failed trials in the Sudakov veto algorithm
  - Validation successful in Z+jets data
- Also DGLAP splitting-kernel uncertainties studied
  - Become negligible when ME corrections are applied
  - Correlation w.r.t. ME uncertainties well understood?
- Not yet used in experiments

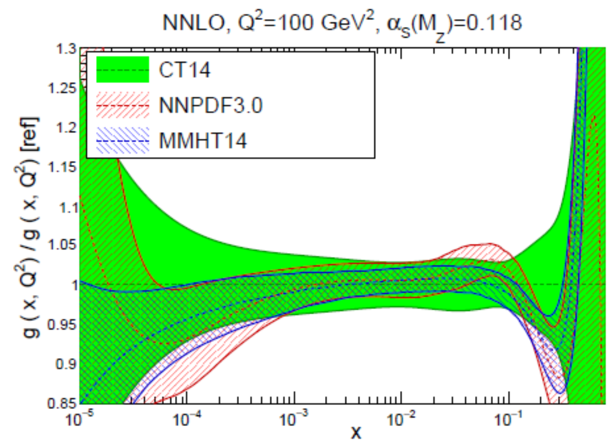


arXiv:1605.08352,
Phys. Rev. D 94, 074005 (2016)

PDFs

- Recent updates (in 2014 and 2017) of PDF fits in collaborations, including LHC data
  - Brought to significantly improved agreement on gluon PDFs
- Recipes used in practice in MC generation
  - Used NNPDF3 (become available first)
  - Store weights for at least:
    - All NNPDF error sets (100 at α_s = 0.118 + 2 α_s variations of +/- 0.001)
    - MMHT and CT
  - NNPDF can be replaced with PDF4LHC15 (preferably with the 100 error set, unless shown that using just the reduced set of 30 makes no difference)
- Of course for precision measurements (e.g. W/Z cross-sections) the recommendation is still to publish giving the result for various PDF sets



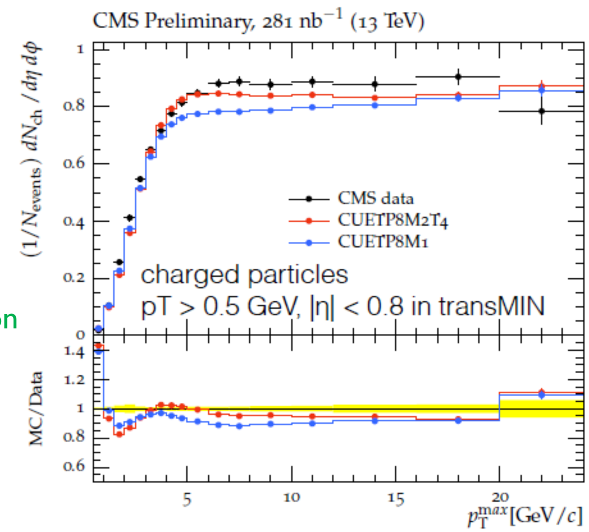


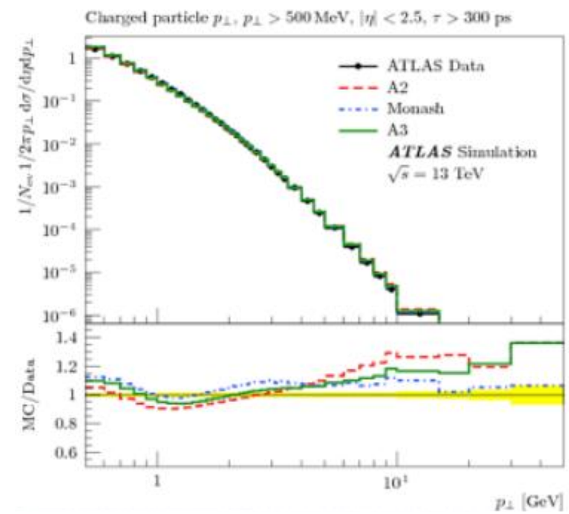
J. Phys. G: Nucl. Part. Phys. 43 023001 (2016)

Underlying event tunes

- Very significant work in both ATLAS and CMS to extract UE (DPS) tunes from Minimum Bias (4-jet, same-sign WW etc.) data

CMS-GEN-17-002, Paper in preparation





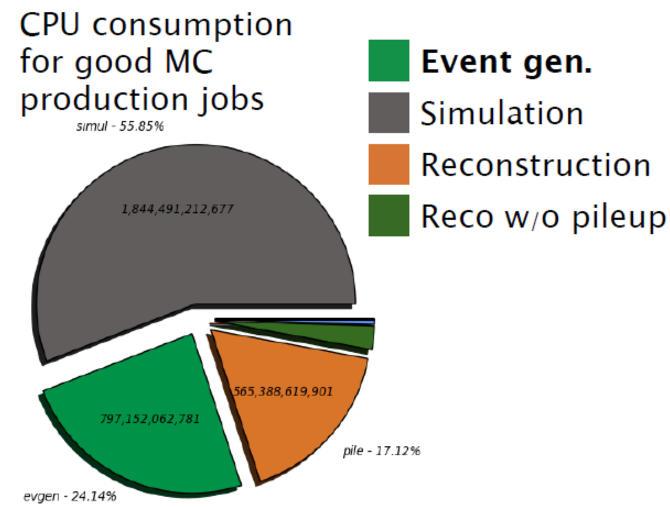
ATL-PHYS-PUB-2017-008

- Uncertainties estimated via «eigentunes»
- Problem: ATLAS/CMS produce MC samples with its own latest version of UE tunes → affects main-sample **and** PU simulation
  - In several cases, leads to impossibility of one-to-one comparisons

Technical aspects

MC production at LHC experiments

- Nowadays, MC «campaigns» (i.e. sets of samples targeting analysis of a specific LHC dataset) have typical sizes of o(10B) events
  - By far, the most CPU-expensive task in LHC computing
  - Ideally, want to keep a MC/data ratio >> 1
- NLO generators changed the paradigm
  - Before: Generation of the physical event has negligible CPU time/memory consumption w.r.t. other simulation steps (e.g. GEANT)
  - Now: Generation of the physical event can take a substantial amount of time/memory and can be impossible w/o some pre-computation steps



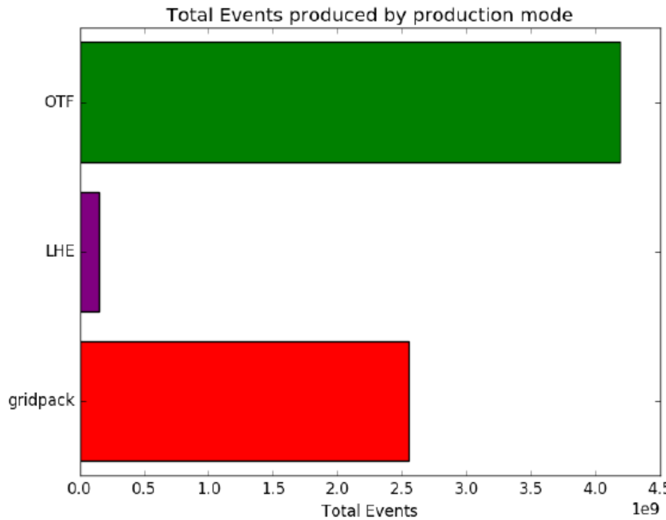
Josh Mc Fayden
@ ATLAS-CMS MC workshop 2016

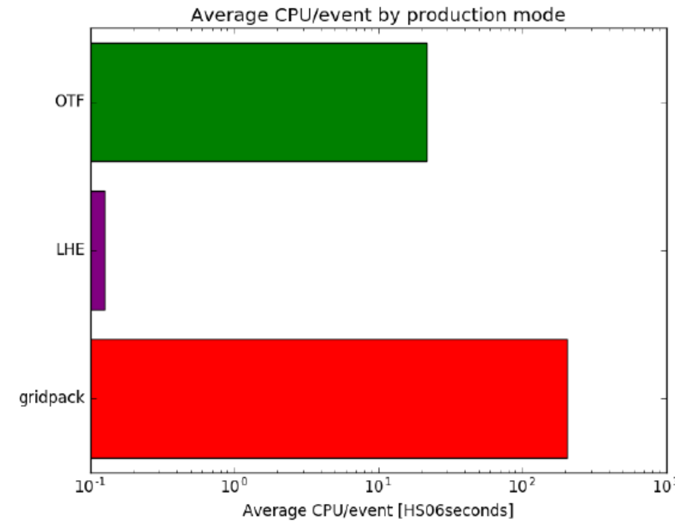
The «gridpack/SHERpack» idea

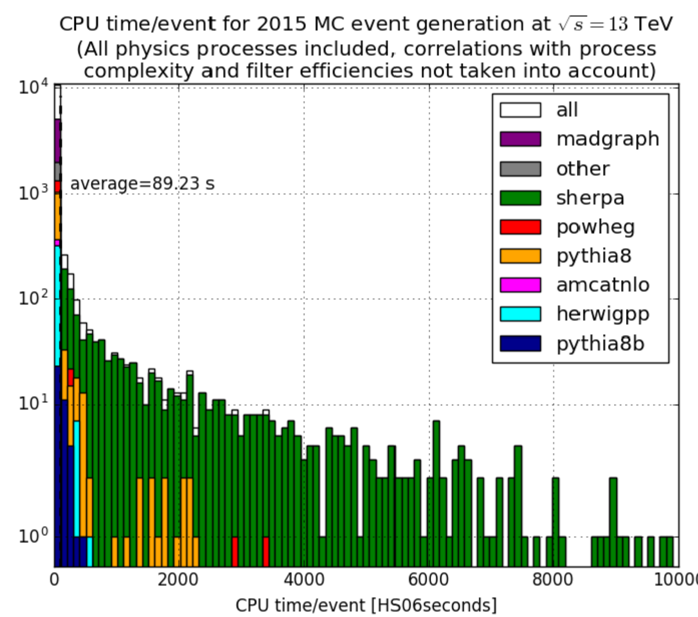
- When event generation is split in several jobs (a must for large generations) there can be some pre-computation steps that are valid once for all, e.g.:
  - Calcualation of diagrams and amplitudes for automated ME generators
  - Optimization of «grids» for MC integration
- Idea: run these steps in advance and store all needed files in a large archive («gridpack») retrieved in each job
  - Code available from authors for MadGraph / SHERPA
  - Written by experimentalists for POWHEG
- **Tested and working**
  - Issue: the «gridpack» creation step does not fit LHC GRID-based computing models
  - Must be performed by a single user using batch queues → can take a long time for NLO processes with high-multiplicity final states

The «gridpack/SHERpack» idea (cont'd)

- RunII MC gridpack use in ATLAS
  - More imbalance vs. gridpacks in CMS
- Time/event split by MC generator in ATLAS
  - Better picture in CMS because of less frequent SHERPA use





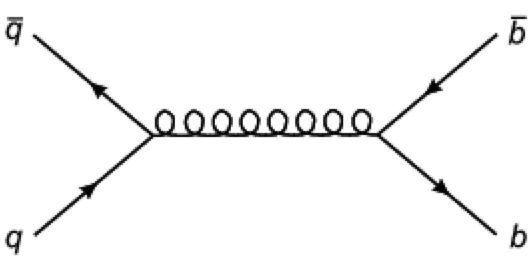


Josh Mc Fayden
@ ATLAS-CMS MC workshop 2016

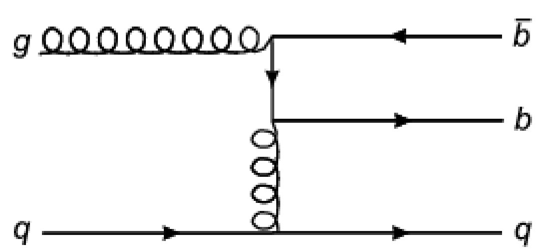
Specific issues for B-physics

- As we discussed in the previous slides, MC for B-physics is typically LO+LL (mostly Pythia)
  - DPS activated inside Pythia to estimate contribution to double Qqbar production
  - Interface to an external decay program (usually EvtGen) is a must for basically the whole set of samples
- Generation of generic QCD is necessary, because the pure pp → Q Qbar generation misses 2 → 3 processes (large σ!) occurring only in subsequent stages of the PS

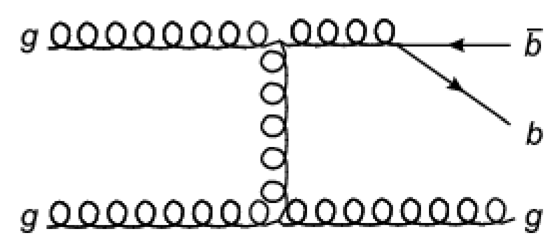
Tree-level



Flavor excitation



Gluon splitting

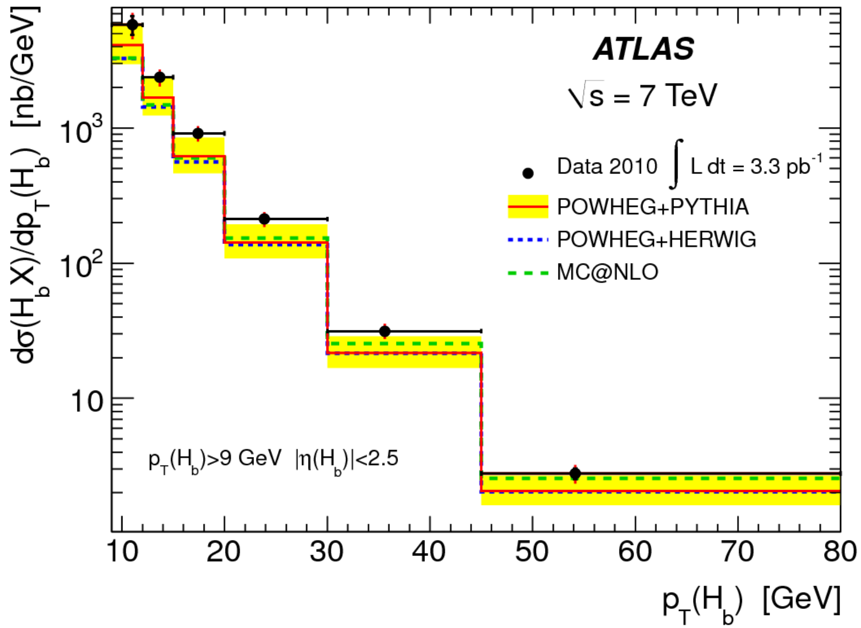


The generation efficiency problem

- Example: generate $B_s \to \mu\mu$ in CMS
  1. Start from generic QCD and find a b bbar pair: $o(10^{-3})$
  2. b or bbar fragmentation into B_s: $o(10^{-1})$
  3. Decay to $\mu\mu$, can be forced in EvtGen: 100%
  4. Muons inside CMS trigger acceptance: $o(10^{-2})$
- Generation efficiency for a detectable event is $o(10^{-6})$
  - Timing of a Pythia8 QCD event is around 10 ms → 10,000 s to obtain a single event, unacceptable for large productions
- Things are even worse for background processes e.g. QCD $\to \mu\mu$, since acceptance is much smaller
- Various workarounds found by experiments
  - Approximate cuts on b-parton kinematics (e.g. not at extreme $|\eta|$)
  - Re-hadronization of events, much faster than producing a new event → Much easier in Pythia8 w.r.t. 6 («UserHooks»)
- Still not a completely settled issue

Moving to NLO?

- NLO generators for pp → Q Qbar available for years
  - And generally used for unfolded data/theory comparisons



- Could not be enough in the description of gluon splitting that can happen at a later stage of the PS
  - In precision measurements where X+b (bbar) is a major background (e.g. VHbb, ttHbb), the recipe is to merge a NLO X+b (bbar) sample with a second sample where LHE-level b's are vetoed and events are filtered on the presence of a b in the PS
  - Does not solve the efficiency problem

Conclusions

- MC-generator evolution showed an impressive rate in recent years
  - Not just in the available tools but also in input parameters (e.g. updated PDFs)
- Not always followed by timely application in experiments
  - Generator-integration or CPU timing issues
  - Limited manpower
  - «Campaign» structure: full set of consistent MC events produced in one shot and then kept for long periods (considering the re-Reco option, can be a few years)
  - Complex applications of theory recipes difficult to incorporate into sample production workflows

Back up