Precision Simulations and their Limitations

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disclaimer (I): I'll focus on challenges for the HL-LHC &

will try to provide an alternative perspective

(my apologies if I miss/misrepresent something dear to your heart) disclaimer (II): I will **not** talk about any specific BSM and/or SMEFT

(my apologies: most "simple" signals under good control)

$\longrightarrow$ imo: HL-LHC = game of SM precision in extreme phase spaces

- introduction
- fixed-order perturbation theory
- better parton showers
- soft physics
- summary

setting the scene

(we theorists did pretty well, didn't we?)

preface: how to build an event generator

- paradigm: "divide et impera"
- divide simulation in distinct phases, with (logarithmically) separated scales
- start with signal event

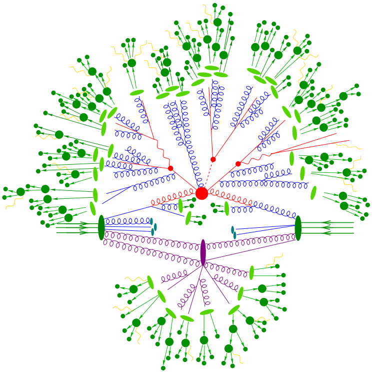
  (fixed order perturbation theory)
- dress partons with parton shower

  (resummed perturbatkon theory)
- add underlying event

  (phenomenological models)
- hadronize partons

  (phenomenological models)
- decay hadrons

  (effective theories, simple symmetries & data)



executive summary: theory precision

(apologies to any paper/author I didn't mention – this is a rich and highly successful & diverse field)

- ✓ $2 \to 1$ scattering processes @ N^{3}LO(QCD)

  (e.g. 1503.06056,)

- ✓ $2 \to 1$ scattering processes @ mixed two-loop QCD$\otimes$ EW

  (e.g. 0811.3458, 2005.10221, 2009.10386, 2203.11237, 2401.15682, ...)

- ✓ $2 \to 2$ scattering processes @ NNLO(QCD)

  (e.g. 1303.6254, 1408.5243, 1408.5325, 1611.01460, 2102.13583, 2105.00954, 2110.12992, 2204.10173, 2311.14991, ..., MCFM)

- ✓ first two-loop **cross sections** and amplitudes for $2 \to 3$ @ NNLO(QCD)

  (e.g. 1310.1051, 1712.02229, **1911.00479**, **2102.02516**, **2105.06940**, **2205.01687**, **2304.06682**, 2404.12325, 2409.08146, ...)

- ✓ $2 \to n$ scattering processes @ NLO(QCD or EW) automated

  (OPENLOOPS/RECOLA +SHERPA, MADGRAPH, MCFM)

- ✓ NNLO+NNLL singlet production

  (e.g. 0705.3887, 1007.2351, 1007.4005, 1109.2109, 1507.02565, 2009.11437, 2210.10724, 2301.11768, ...)

executive summary: Monte Carlo perturbative precision

- ✓ NNLO ⊗ parton shower for colour singlet production

  (MINNLO: 1309.4634, 1407.2940, . . . , 2208.12660; UNNLOPS: 1405.4607, 1407.3773)

- ✓ NNLO ⊗ parton shower for heavy quarks

  (MINNLO: 2112.04168 ($t\bar{t}$), 2302.01645 ($b\bar{b}$))

- ✓ MEPS@NLO: NLO multijet merging

  (SHERPA: 1207.5030; MADGRAPH: 1209.6215; PYTHIA: 1211.7278; HERWIG: 1705.06700 plus follow-ups & refinements)

- ✓ all of the above including EW@NLO

  (explicit: 1511.08692, 1705.00598, . . . , 2204.07652; Sudakov approximation: hep-ph/0010201, 2111.13453)

- ✓ (N)NLO ⊗ N^{1,2,3}LL⊗ parton shower

  (GENEVA: 1211.7049, 1508.01475, 2102.08390, . . .)

- ▶ improving parton showers

  ((next-to leading) logarithmic accuracy (see below); amplitude evolution: 1802.08531, . . . (not covered here))

- ▶ multijet merging with TMDs (2107.01224, 2208.02276 (not covered here))

fixed-order perturbation theory

(challenges in the race for more N's)

current technical bottlenecks: an outsider's view

(I am sure I misrepresent some details . . . – however, I am sure they will all be solved)

- two-loop virtual terms for $2 \to n$:
  complexity of integral basis explodes with number of scales

  (and their evaluation involves costly special functions or intricate numerics)

  $\longrightarrow$ work in progress (see some of the $2 \to 3$ papers above)
- often overlooked: stability of $2 \to n+1$ one-loop virtuals:
  (semi-)automated numerical methods may not be good enough
  $\longrightarrow$ need analytical solutions (?)
- NNLO subtraction terms - plethora of methods/algorithms

  (remember: "NLO revolution" due to mix of generic virtuals + automated real subtraction)

  $\longrightarrow$ work in progress

  (recent and not so recent: hep-ph/0609042, 1505.04794, 1702.01352, 1806.09570, 1902.02081, 2203.13531, 2310.17598, 2310.19757, 2403.03078, . . .)

other challenges

(. . . and I have no idea how to address them systematically)

- sociological: increasingly forbidding learning threshold

  $\longrightarrow$ increasingly difficult start for new PhD students

- conceptual (I): breakdown of factorisation at $\mathcal{O}(\alpha_S^N)$ (1112.4405, 1206.6363)

  ✓ pure QCD at two-loop

  ✗ non-cancellation of Coulomb effects at three loops for non-inclusive QCD observables $\longrightarrow$ "super-leading logs"
  but: possibly restored through Glauber gluons (2408.10308)

  $\longrightarrow$ introduces possible process/observable dependence

- conceptual (II): factorisation assumes terms Λ/Q can be ignored

  (where Λ is soft, Q is hard scale, no guarantee that "higher-twist" comes quadratically)

  - size-estimate for Drell-Yan: $Q \approx 100$ GeV, Λ? . . .

$\longrightarrow$ how much do higher-twist corrections contribute to uncertainty?

better parton showers?

(the story never gets old – at least to me)

why do we care?

- recent concerns about their logarithmic accuracy

  (theoretically dissatisfying, although data description ok so far)

- want to assess related theory uncertainty

  (traditional scale variation pointless without h.o. compensating terms)

- process-independent NNLO matching: need $\mathcal{O}(\alpha_S^2)$ splitting kernels

  (which are also crucial for NNLL accuracy)

- establish links with analytic resummation

  (and differences due to finite recoils etc.)

a new parton shower for SHERPA

(2208.06057, 2404.14360)

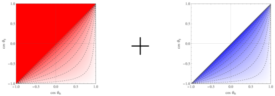
- **positive definite** soft-eikonal decomposition (**new**, allows simple prob. interpretation):

  (borrowing from Catani & Seymour, Nucl. Phys. **B485** (1997) 291)
- match with collinear terms
- introduce **new** kinematics:
  colour-spectator $\neq$ recoil partner

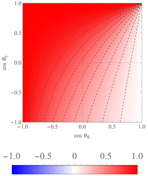
  (highly flexible, allows for uncertainty estimates due to kinematics)
- (first) analytic proof of NLL accuracy & extensive numerical tests
- (first) multi-jet-merging at LO
- bespoke NLO subtraction scheme
  ($\rightarrow$ seamless MC@NLO/MEPS@NLO)

  (currently being implemented & validated)

- usual decomposition:

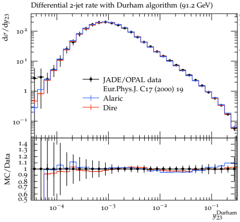


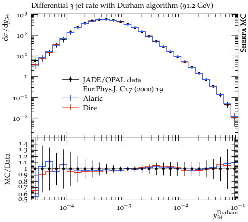
- new decomposition:

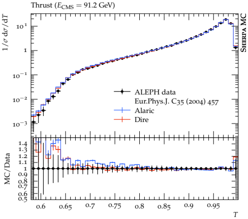


some example results

- precision LEP results ($\alpha_S = 0.118$, no merging)

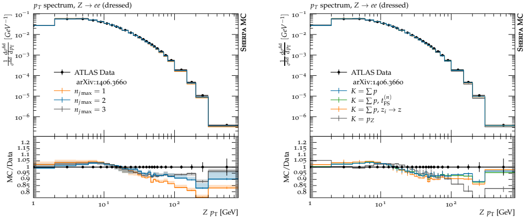






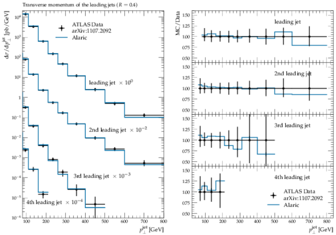
some example results

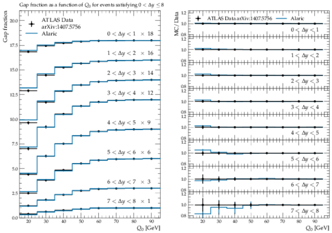
- precision Drell-Yan @ LHC results (α_S from PDFs, merging)



some example results

- jets @ LHC results (α_S from PDFs, with merging)





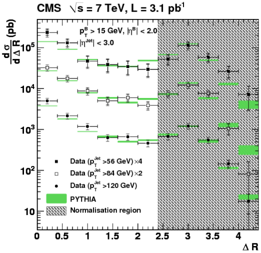
challenge: $g \to Q\bar{Q}$ in the final state

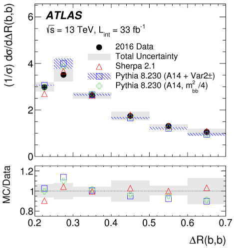
- parton showers geared towards collinear & soft emissions of gluons

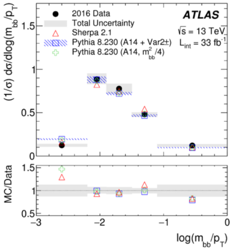
  (double log structure)

- $g \to q\bar{q}$ only collinear, subtle phase space
- questions: kernel, scale in α_s: fix this with theory + LHC data

  (important for $t\bar{t}b\bar{b}$, boosted H, $H + c$, $V + c$, dots)





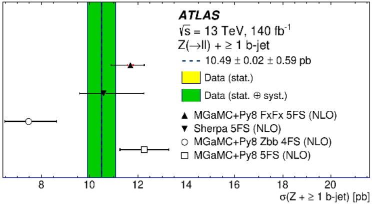


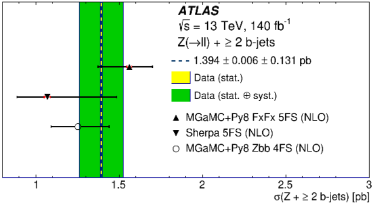
massive quarks in the initial state

(see, e.g., 2403.15093)

- associated production of heavy quarks: 4F vs. 5F scheme

(large uncertainty in $Z+b$, $t\bar{t}b\bar{b}$, ...)





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(see, e.g., 2205.02817)

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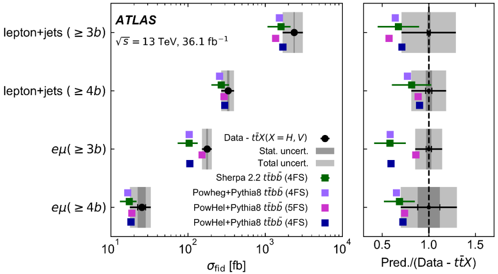
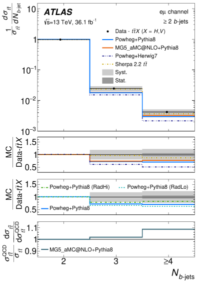




massive quarks in the initial state

- associated production of heavy quarks: 4F vs. 5F scheme

  (large uncertainty in $Z+b$, $t\bar{t}b\bar{b}$, ...)
- for 5F: need heavy quarks in initial state $\longrightarrow$ problematic

  $\longrightarrow$ tricky for (N)NLO calculations including m_Q: subtraction terms

  $\longrightarrow$ no PDF support for $Q^2 \leq m_Q^2$ $\longrightarrow$ quarks stop showering
- possible solutions:
  - naive: ignore and leave for beam remnants (Sherpa)
  - better: enforce splitting in region around m_Q^2 (Pythia)

    $\longrightarrow$ effectively produces collinear Q and gluon in IS
- will need to check effect on precision observables: $p_\perp^{(W)}/p_\perp^{(Z)}$

challenges

(I am quietly confident most of them will be solved)

- practical: going beyond NLL
  $\longrightarrow$maintaining positivty $\longleftrightarrow$ probabilistic interpretation
  (this is one of the nice features of parton showers)
- conceptual (I): maintaining/pushing precision
  $\longrightarrow$matching with fixed-order (NNLO!) for arbitrary processes
  (need to fully & analytically understand double emission phase space)
- conceptual (II): assessing precision
  $\longrightarrow$need a way to systematize this
  (scales, kinematics/recoil schemes, interface to hadronization, ...)
- sociological: increasingly forbidding learning threshold
  $\longrightarrow$ increasingly difficult start for new PhD students (most event generators turned into massive software projects)

soft physics

(the elephant in the room)

higher twist: (hard) double parton scattering (DPS)

- example: same-sign W-pair production
  - interesting final state, probes lots of gauge structures
    - EW $\approx$ QCD, $qq' \to \tilde{q}\tilde{q}' W^\pm W^\pm$ finite $\forall p_\perp^q$
    - no need to tag forward jets – different to backgrounds
  - but: $\sigma_{\rm direct} \approx \sigma_{DPS}$, double-parton scattering

supreme testing ground for double-parton scattering

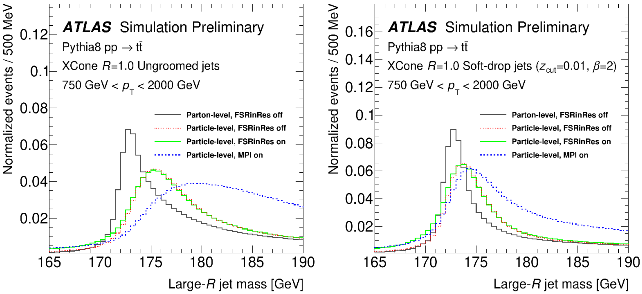
- DPS significant in many other processes (e.g. Wjj production), effect more pronounced in certain phase spaces
- first steps towards first-principles understanding of DPS and its interplay with multi-parton PDFs

(see e.g. 1708.03528, 2305.09716, . . .)

(multi-parton PDF DGLAP evolution tend to ignore impact of spatial distance)

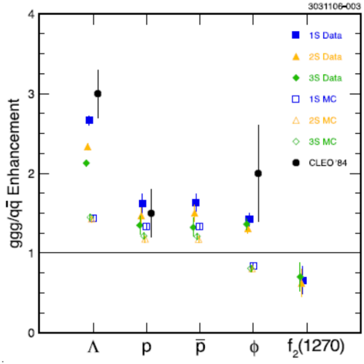
higher twist: multi-parton interactions (MPIs)

- even without **really** hard secondary scatters: clear evidence for MPIs
  - due to proton = extended objects, contain multiple partons
  - overall: deposit energy/particles everywhere, change jet shapes
- example: impact on top mass in boosted tops (below, from ATL-PHYS-PUB-2021-034)



a potential hadronization issue: gluon fragmentation

(from 0704.2766, just an example for more issues)



- tunes dominated by LEP 1

  (10M Z events are hard to argue with)

- but: mainly quarks
- to have handle on gluons: flavour-tagged Mercedes-star events

  (they are rare!)

- alternatively: decays of vector mesons $(Q\bar{Q})$ (see right)

  (either $V \to ggg$ (QCD) or $V \to f\bar{f}$ (QED))

- issues with strangeness/baryons?

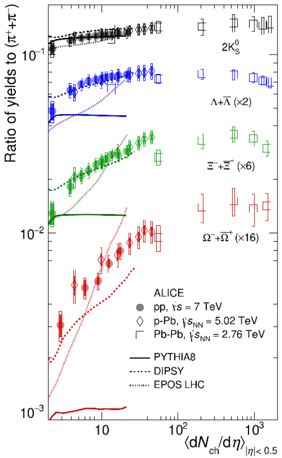
hadronization issues: strange strangeness

- models date back to the 1970's/80's based on
  - linear QCD potential (strings) or
  - Local Parton Hadron Duality (clusters)
- hadronization universality **assumed**
- parameters tuned to LEP data
  in particular: strangeness suppression
- for strangeness: **flat ratios** in the "usual" multi-purpose MC's
  but data do not reproduce this

  needs "colour ropes" or some such

- looks like $SU(3)$ restoration
  not observed for protons

(from 1606.07424, just another example for more issues)

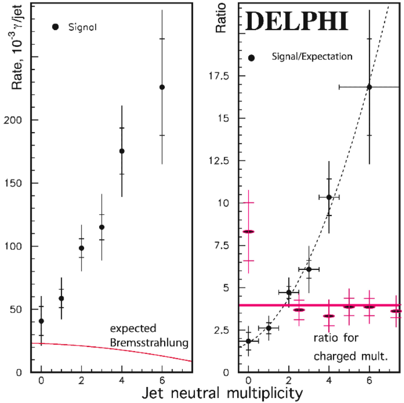


another thing that doesn't work: soft photons

(from 1004.1587)

- DELPHI expectation:
  0.02 soft photons/jet flat
  (dependent on isolation cuts)
- but: strong scaling with neutral hadron multiplicity (see right)
- possible explanations:
  - (magnetic) dipole emissions?
  - enhanced radiation off quarks during hadronization?
  - . . .

so far unable to reproduce data



another nuisance: colour reconnections

(they certainly exist – implementation through various ad-hoc models)

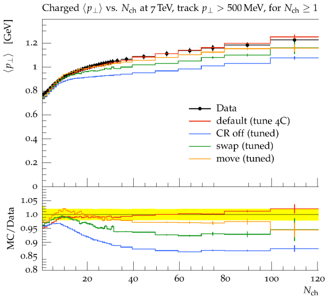
- origins of colour reconnections:
  - $N_c = 3$ vs. $N_c \to \infty$

    (used in parton showers)
  - soft, non-perturbative "gluers"
- modelling colour reconnections:
  - reshuffle colours after parton shower

    (exhibiting non-pert. nature)
  - "shuffle" probabilities based on phase-space distances
- models quite ad-hoc

  first-principles models needed!

- effect on particle spectra in MinBias:



(from 1407.6653)

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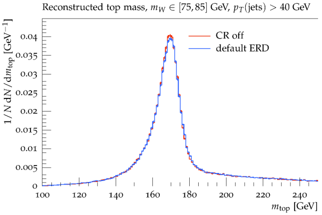
  first-principles models needed!

- effect on $m_{\rm top}$:

  $\Delta m_{\rm top} \approx \pm\Lambda_{QCD}$

  (see, e.g., 1810.01772)



(from 1407.6653)

yet another nuisance: Bose–Einstein correlations

(they certainly exist – so far only ad-hoc models in PYTHIA)

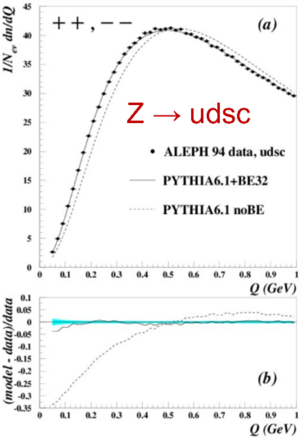
- quantum statistics of identical particles

  (produced at "same" point)

- effect: identical particles i and j "want" to be closer in phase space closeness parametrised by $Q^2 = -(p_i - p_j)^2$
- correlation function $f_2(Q^2) = 1 + \lambda \exp(-Q^2 R^2)$

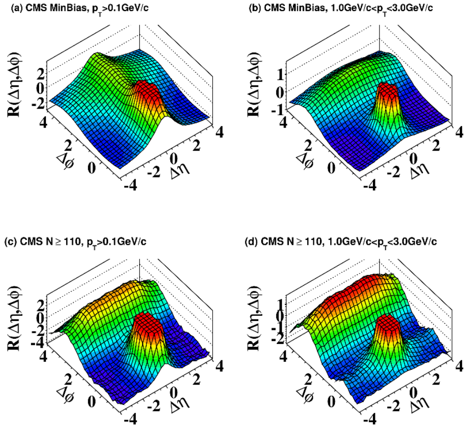
  (with $\lambda \sim 1$, $R \sim 0.5$ fm)

- so far only implemented in PYTHIA as phenomenological "after-burner" by shifting hadron momenta



unsolved: the emergence of collectivity

(from 1009.4122, I am not aware of any genuine first-principles solution)



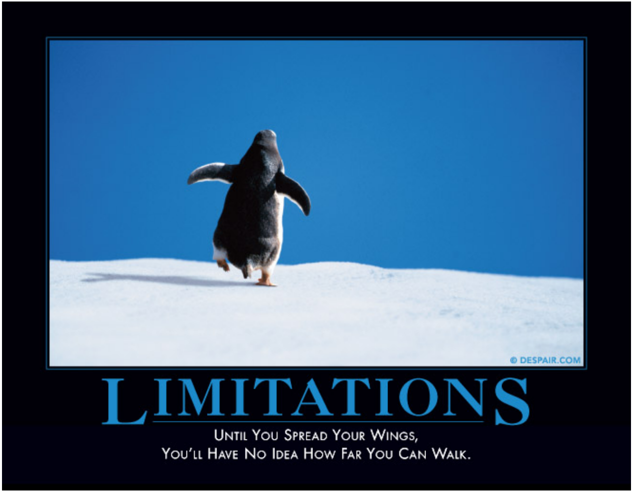
summary

my prediction: future "attractions"

- solvable (and probably solved within the decade):
  practically everything at the precision frontier
  - NNLO (QCD) for $2 \to n$ processes
  - (N)NLL parton showers and their matching to NNLO
  - two-loop mixed QCD $\otimes$ EW for $2 \to 2$ processes
- extremely tricky (and probably not solved within the decade):
  practically everything with non-perturbative physics
  main obstacles:
  - lack of people power – not attractive for ECRs
  - lack of compelling ideas
  - absence of systematic treatment ("eigen-tunes")):
    perception of sufficient approach to extracting non-pert. uncertainties by merely "flicking" through tunes

final thoughts

- perception/common narrative (I):
  HL-LHC and results are a "done deal" – certainly overly naive!
  (still a lot of work to be done – conceptually, methodologically, implementation, validation, . . .)
- perception/common narrative (II):
  higher theoretical accuracy $\leftrightarrow$ decreasing experimental uncertainties
  (this reduces theory to indispensable help for experimental data analysis)
- challenge reductionist approach:
  which new things can we learn/decipher with precision?
  ("rediscover" precision theory as input to design of new analyses/measurements)
- also: is there something beyond "more N's"?
  we may want/need to look at non-perturbative effects
  (it is conceivable that they may become the largest impediment for theory accuracy for some measurements)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LIMITATIONS
Until You Spread Your Wings,
You'll Have No Idea How Far You Can Walk.