

# Monte Carlo challenges for the future

Stefan Höche

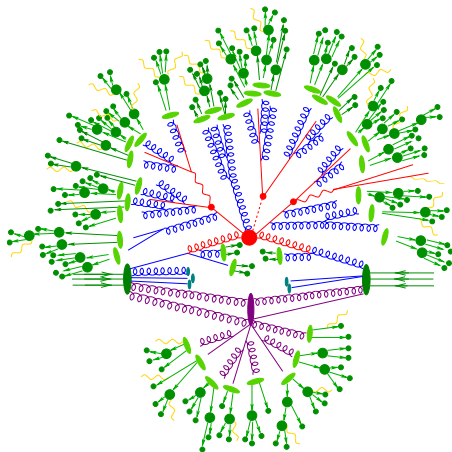
Fermilab

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# State of the art

- ▶ LO Matrix Element generators and Loop-ME Generators
- ▶ Parton showers, mostly based on dipole/antenna picture
- ▶ Multiple interaction models possibly interleaved with shower
- ▶ Hadronization models string/cluster fragmentation
- ▶ Hadron decay packages
- ▶ Photon emission generators YFS formalism or QED shower



**Much of the development focused on increase in perturbative precision**

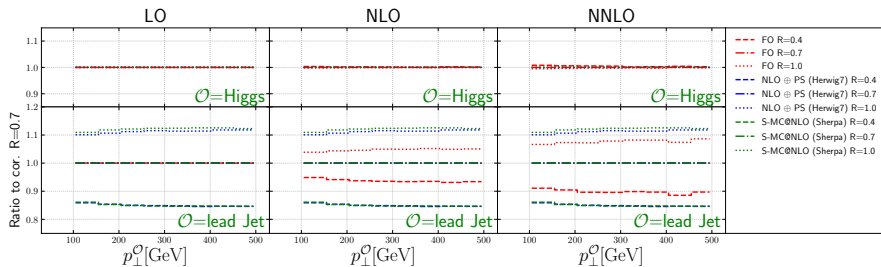
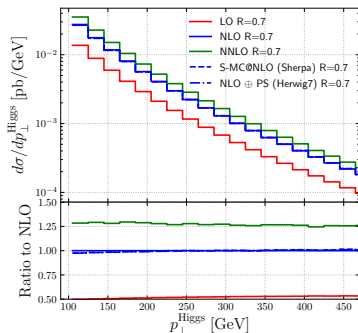
→ Incorporation of higher orders in  $\alpha_s$ ,  $\alpha_s L$ ,  $1/N_c$ , ... expansion while maintaining local, fully differential event generation paradigm

**This talk: A sample of results and developments, and a (biased) outlook**

# Where do we stand? N<sup>(2)</sup>LO / MC comparison in gg→Hj

[Bellm et al.] arXiv:1903.12563

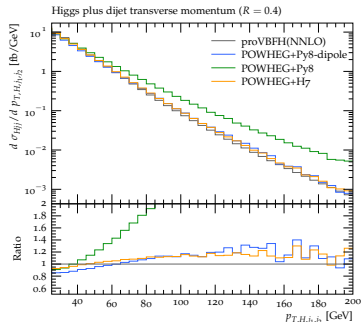
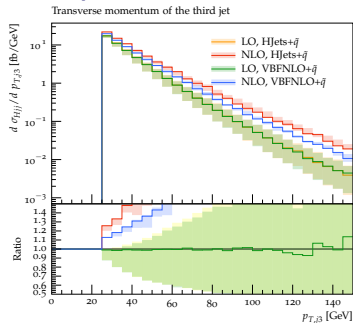
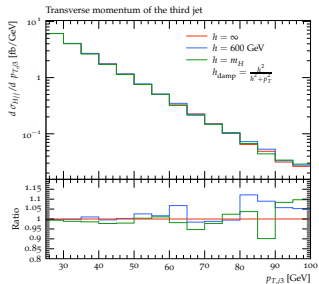
- ▶ Good agreement between MC@NLO (Herwig / Sherpa) and fixed-order pQCD for inclusive observables in  $pp \rightarrow Hj$
- ▶ Radius dependence of cross section well modeled by MC in comparison to NNLO
- ▶ Spurious reduction of uncertainties at small R, more pronounced at NNLO than NLO → alternative prescription needed, e.g. [Dasgupta,Dreyer,Salam,Soyez] arXiv:1602.01110



# Where do we stand? N<sup>(2)</sup>LO / MC comparison in VBF

[Jäger,Scheller,Plätzer,Karlberg,Zaro] arXiv:2003.12435

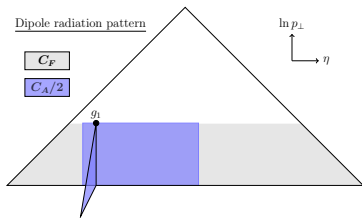
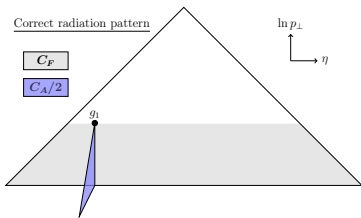
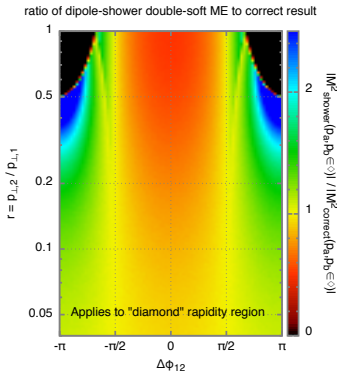
- ▶ Comparison between common tools Herwig/HJets, POWHEG/Pythia, and fixed-order NNLO
- ▶ Uncertainties of order 10% for more inclusive observables, order 20% for observables sensitive to radiative effects
- ▶ VBF process quite insensitive to form of Sudakov in POWHEG-BOX → little impact of  $h_{\text{damp}}$  parameter



# Parton showers beyond LL accuracy

[Dasgupta,Dreyer,Hamilton,Monni,Salam] arXiv:1805.09327

- ▶ Two problems in commonly used parton showers when compared to analytic NLL resummation:
  - ▶ Angular correlations across multiple emissions due to recoil strategy and choice of evolution variable spoil accuracy
  - ▶ Average color charge of initial  $q\bar{q}$  dipole after radiation not reflected correctly in commonly used dipole shower approaches
- ▶ Both issues in strongly ordered soft limit



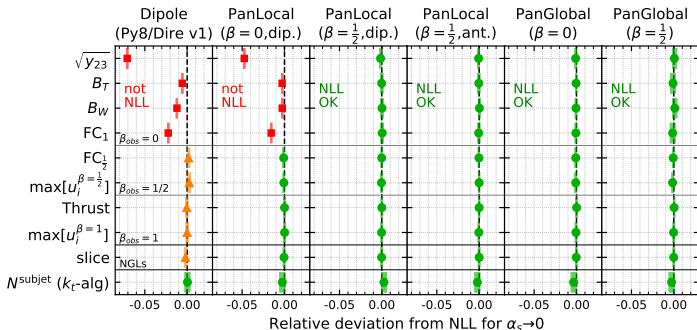
# Parton showers beyond LL accuracy

[Dasgupta,Dreyer,Hamilton,Monni,Salam,Soyez] arXiv:2002.11114

- Both problems solved by partitioning of antenna radiation pattern and choosing a suitable evolution variable ( $\beta \sim 1/2$ )

$$k_T = \rho v e^{\beta|\bar{\eta}|} \quad \rho = \left( \frac{s_i s_j}{Q^2 s_{ij}} \right)^{\beta/2}$$

- Three different recoil schemes lead to NLL result if  $\beta$  chosen appropriately: Local dipole, local antenna, and global antenna
- First provably NLL correct parton shower for  $e^+e^- \rightarrow \text{hadrons}$



# Towards parton showers at NLO

- Collinear limit: Higher-order DGLAP kernels obtained by factorization

$$D_{ji}^{(0)}(z, \mu) = \delta_{ij} \delta(1-z) \quad \leftrightarrow \quad \text{[Diagram: Circle with incoming line } j \text{ and outgoing line } z \text{]} / \text{[Diagram: Circle with incoming line } i \text{ and outgoing line } 1 \text{]}$$

$$D_{ji}^{(1)}(z, \mu) = -\frac{1}{\epsilon} P_{ji}^{(0)}(z) \quad \leftrightarrow \quad \text{[Diagram: Circle with incoming line } i \text{ and outgoing line } z \text{, with a gluon emission from the vertex]} / \text{[Diagram: Circle with incoming line } i \text{ and outgoing line } 1 \text{]}$$

$$D_{ji}^{(2)}(z, \mu) = -\frac{1}{2\epsilon} P_{ji}^{(1)}(z) + \frac{\beta_0}{4\epsilon^2} P_{ji}^{(0)}(z) + \frac{1}{2\epsilon^2} \int_z^1 \frac{dx}{x} P_{jk}^{(0)}(x) P_{ki}^{(0)}(z/x)$$

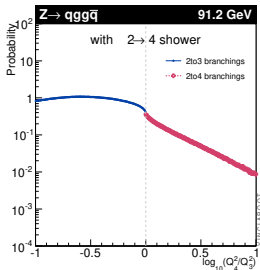
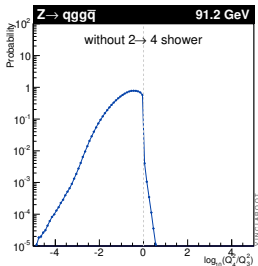
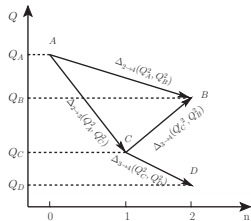
$$\leftrightarrow \left( \text{[Diagram: Circle with incoming line } i \text{ and outgoing line } z \text{, with a gluon emission from the vertex]} + \text{[Diagram: Circle with incoming line } i \text{ and outgoing line } z \text{, with a gluon emission from the vertex]} \right) / \text{[Diagram: Circle with incoming line } i \text{ and outgoing line } 1 \text{]}$$

- Being able to compute  $P_{ji}^{(1)}$  fully differentially in the parton shower is a prerequisite for NNLL accuracy in an observable-independent way
- $P_{ji}^{(1)}$  not probabilities, but sum rules hold ( $\leftrightarrow$  unitarity constraint)  
In particular: Momentum sum rule identical between LO & NLO
- Soft limit schematically identical, but beware of overlap with collinear!

# Towards parton showers at NLO

[Hartgring,Laenen,Skands] arXiv:1303.4974, [Li,Skands] arXiv:1611.00013

- ▶ ME-corrected showers (e.g. Vincia) predict correct 2-emission pattern  $\rightarrow$  possibility to extend to full NLO by including virtual corrections
- ▶ Result depends on evolution variable due to phase-space restrictions in real emission integrals that arise from ordering (e.g.  $A \rightarrow B \rightarrow C$ )
- ▶ If missing phase space region is filled by direct  $2 \rightarrow 4$  transitions ( $A \rightarrow B$ ) obtain complete NLO antenna shower framework



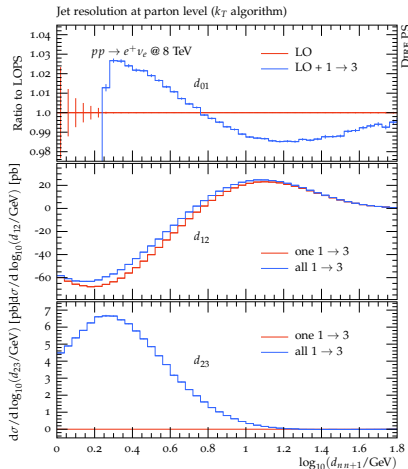


# Towards parton showers at NLO

- ▶ Alternative approach based on standard parton shower:
  - ▶ Subtracted  $2 \rightarrow 4$  splitting function in ordered phase-space region
  - ▶ Complete  $2 \rightarrow 4$  splitting function in unordered phase-space region
- ▶ Structurally identical to fixed-order subtraction (e.g. Catani-Seymour)

$$P_{qq'}^{(1)}(z) = C_{qq'}(z) + I_{qq'}(z) + \int d\Phi_{+1} \left[ R_{qq'}(z, \Phi_{+1}) - S_{qq'}(z, \Phi_{+1}) \right]$$

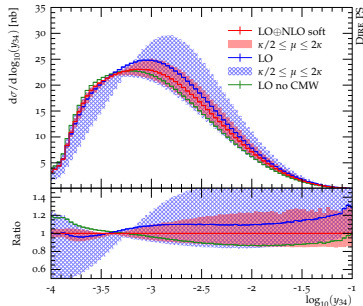
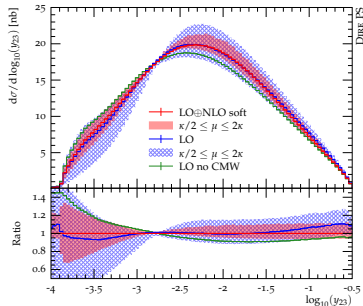
- ▶ Shown to reproduce known NLO splitting functions in collinear limit  
[Curci,Furmanski,Petronzio] NPB175(1980)27



# Towards parton showers at NLO

[Dulat,Prestel,SH] arXiv:1805.03757

- ▶ Alternative approach for soft radiation
  - ▶ ME correction implements kinematic corrections, angular correlations and first non-trivial sub-leading color contributions
  - ▶ Complete  $2 \rightarrow 4$  splitting function in unordered phase-space region
- ▶ Reproduces benchmark given by soft gluon resummation at 2 loops  
[Belitsky] hep-ph/9808389
- ▶ CMW factor generated differentially by endpoint contributions, yields good agreement with inclusive CMW scheme

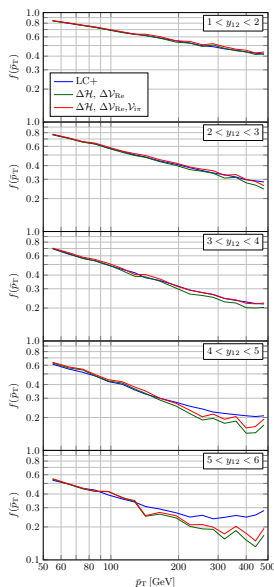


# Parton showers beyond LC accuracy

[Nagy,Soper] arXiv:1902.02105, arXiv:1905.07176

- ▶ Systematic expansion of shower operator acting on statistical space
- ▶ Starts with LC+ approximation  $\rightarrow$  simplify color insertion operators  $T_i T_k \rightarrow T_i^2$  but retain bra/ket states exactly
- ▶ Extension to higher number of terms in  $1/N_c$  by means of additional operators
  - ▶  $\Delta\mathcal{H}$  - real-emission
  - ▶  $\Delta\mathcal{V}_{Re}$  - virtual correction (real part)
  - ▶  $\mathcal{V}_{i\pi}$  - virtual correction (imaginary part)
- ▶ Threshold resummation possible

[Nagy,Soper] arXiv:1711.02369

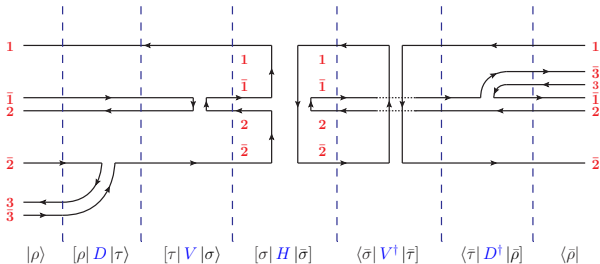
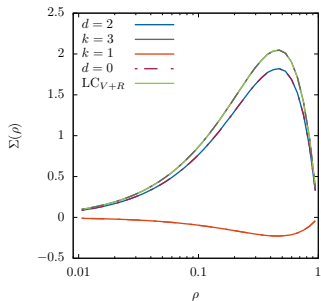


# Parton showers beyond LC accuracy

[DeAngelis,Forshaw,Plätzer] arXiv:2007.09648

- ▶ Amplitude based evolution using color flow decomposition
- ▶ Systematic expansion in  $1/N_c$  terms related to number of swaps of color lines

singlet  $\rightarrow gg$   $N^k$  composition at  $n = 1$

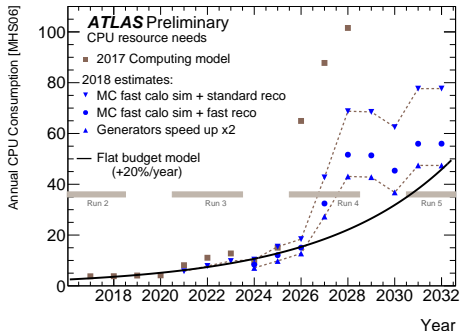
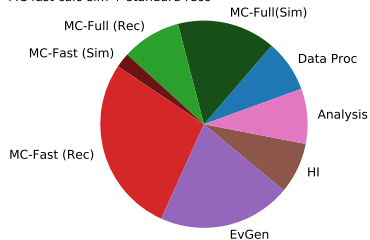


# Computing challenges

[HSF Generator WG] arXiv:2001.10028

- ▶ Event generation will consume significant fraction of resources at LHC soon
- ▶ Need to scrutinize both generator usage and underlying algorithms
- ▶ Dedicated effort in HEP Software Foundation (HSF)

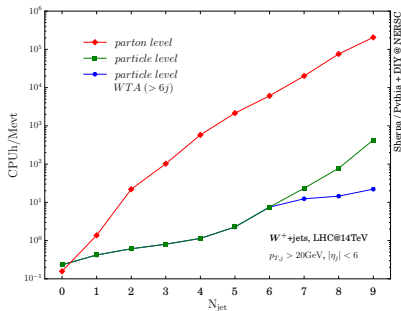
**ATLAS Preliminary. 2028 CPU resource needs**  
MC fast calo sim + standard reco



[ATLAS] <https://twiki.cern.ch/twiki/bin/view/AtlasPublic/ComputingandSoftwarePublicResults>

# Computing challenges

- ▶ Hard scattering simulation much more demanding than parton shower & hadronization in multi-jet merged simulations
- ▶ Complexity of merging ME&PS grows quickly due to inherent  $N!$  scaling of algorithms, but still negligible compared to hard scattering calculation



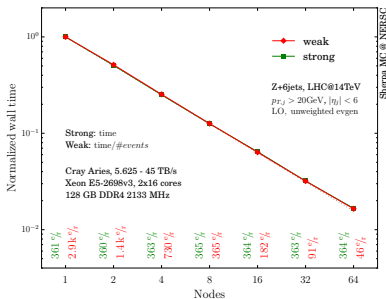
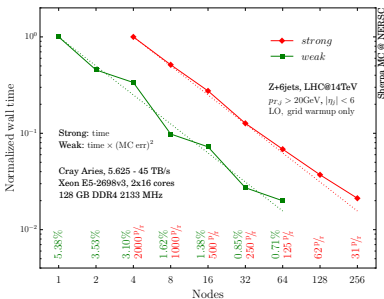
## Origin of the problem

- ▶ Best case ME computation naively scales as  $\approx \mathcal{O}(3^N)$
- ▶ Monte-Carlo unweighting efficiency degrades quickly due to high dimensionality of phase-space integral ( $3N-4$ )
- ▶ Overall scaling  $\approx \mathcal{O}(4^N)$  if not taking cuts into account
- ▶ Cut inefficiencies worsen the picture significantly

# Parallel computing

[Prestel,Schulz,SH] arXiv:1905.05120

- ▶ Integration / event generation performed on multiple cores
- ▶ Vegas grid warmup step scales (strong & weak) up to  $\sim 2048$  cores
- ▶ Event generation step scales (strong & weak) up to  $\sim 2048$  cores
- ▶ Performance limited by number of events being processed per rank (Average timing can only be expected if statistics is large enough)



# Improved NLO matching

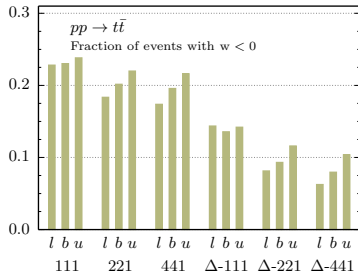
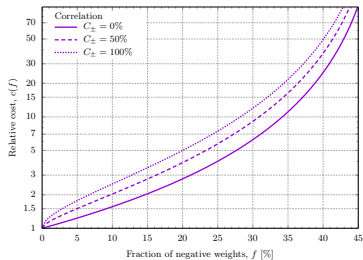
[Frederix,Frixione,Prestel,Torrielli] arXiv:2002.12716

- ▶ For NLO matched simulations, efficiency largely depends on negative weight fraction in hard cross section calculation
- ▶ Negative weights can be significantly reduced by performing partial merging, schematically

$$\mathbb{H} \rightarrow (R - S)\Delta$$

$$\mathbb{S} \rightarrow B + V + I + \int S\Delta + \int R(1 - \Delta)$$

- ▶ Convergence of additional contribution to  $\mathbb{S}$ -events can be improved by folding

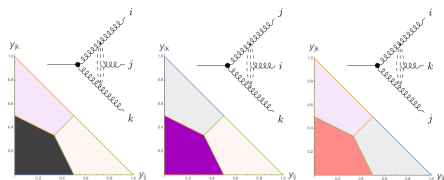




# Sectorization

[Brooks,Preuss,Skands] arXiv:2003.00702

- ▶ Renewed interest in sector showers using antenna approach
- ▶ May provide avenue to more efficient merging due to unique branching history
- ▶ Novel implementation of algorithm in Vincia for hadron colliders and decays [Brooks,Skands] arXiv:1907.08980



	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$
CS Dipole	2	8	48	384	3840	46080	645120
Global Antenna	1	2	6	24	120	720	5040

# Summary

- ▶ Good agreement between different MC generators when using similar setups / assumptions
- ▶ NLL accurate evolution → direct comparison to analytic resummation
- ▶ NLO accurate evolution → first realistic uncertainty estimates  
Pathway to observable-independent, NNLL accurate resummation
- ▶ Sub-leading color evolution → improved predictions for processes with high jet multiplicity
  
- ▶ Most of the above improvements imply a certain fraction of negative weights or some other compute inefficiency
- ▶ It is possible that the theoretically improved MCs we desire will not be the tools to produce events for full simulation
- ▶ We might instead want to think about how to calibrate lower-precision (NLO+NLL,LC) MCs with higher-precision (NNLO+NNLL(?),NLC(?)) and then propagate uncertainty predictions