

MC Event Generators and Phenomenology

With a special focus on DIS

Stefan Höche

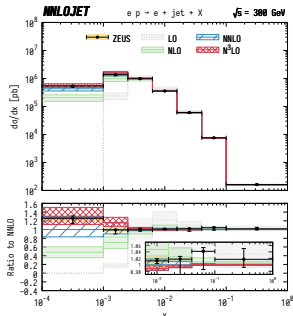
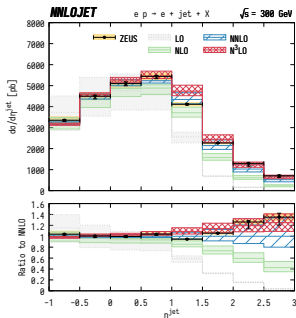
Fermi National Accelerator Laboratory

DIS 2021

Virtual @ Stony Brook, 04/12/2021

DIS as a precision test of QCD

- Inclusive DIS at NLO QCD
[Bardeen,Buras,Duke,Muta] PRD18(1978)3998
[Altarelli,Ellis,Martinelli] NPB143(1978)521
[Humpert,van Neerven] NPB184(1981)225
- ... at N²LO QCD [Zijlstra,vanNeerven]
NPB383(1992)525, PLB297(1992)377
[Moch,Vermaseren] hep-ph/9912355
- ... at N³LO QCD [Moch,Vermaseren,Vogt]
hep-ph/0504242, arXiv:0812.4168
- Di-jet production at NLO QCD
[Mirkes,Zeppenfeld] hep-ph/9511448
[Graudenz] hep-ph/9710244
[Nagy,Trocsanyi] hep-ph/0104315
- ... at N²LO QCD
[Abelof,Boughezal,Liu,Petriello] arXiv:1607.04921
[Currie,Gehrmann,Niehues] arXiv:1606.03991
[Currie,Gehrmann,Huss,Niehues] arXiv:1703.05977
- DIS at N³LO QCD, fully exclusive
[Currie,Gehrmann,Glover,Huss,Niehues,Vogt]
arXiv:1803.09973



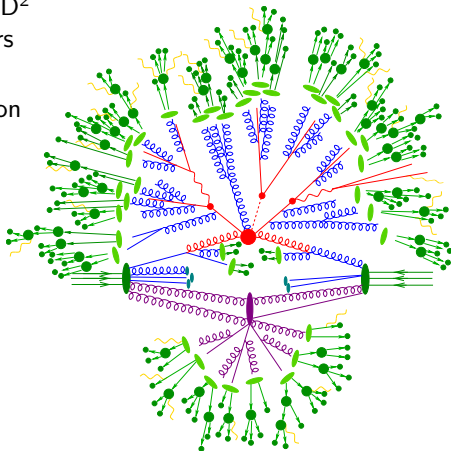
Fixed-order calculations vs event generators

Anatomy of MC simulations

- ▶ **Hard interaction**
LO, NLO QCD/EW¹, NNLO QCD²
Generic matrix-element generators
- ▶ **Radiative corrections**
Parton Showers, YFS resummation
- ▶ **Hadronization & Decays**
Cluster / String model
Phase space or EFTs + YFS

Comparison to fixed order (FO)

- ▶ **Hard interaction**
Lower precision than FO
- ▶ **Radiative corrections**
Resummed & matched to FO
- ▶ **Hadronization & Decays**
Not accessible at FO



¹via interfaces to 1-loop generators

²for selected processes

DIS as a precision test of QCD dynamics

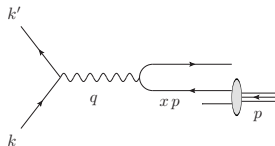
- Inclusive DIS, computed in collinear factorization

- Just a form factor! Described by

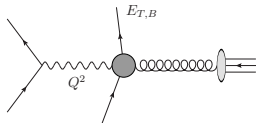
$$Q^2 = q^2 = (k' - k)^2 \text{ and } x = \frac{Q^2}{2q \cdot p}$$

- Hadronic cm energy

$$W = Q\sqrt{(1-x)/x}$$



- QCD dynamics in more differential measurements

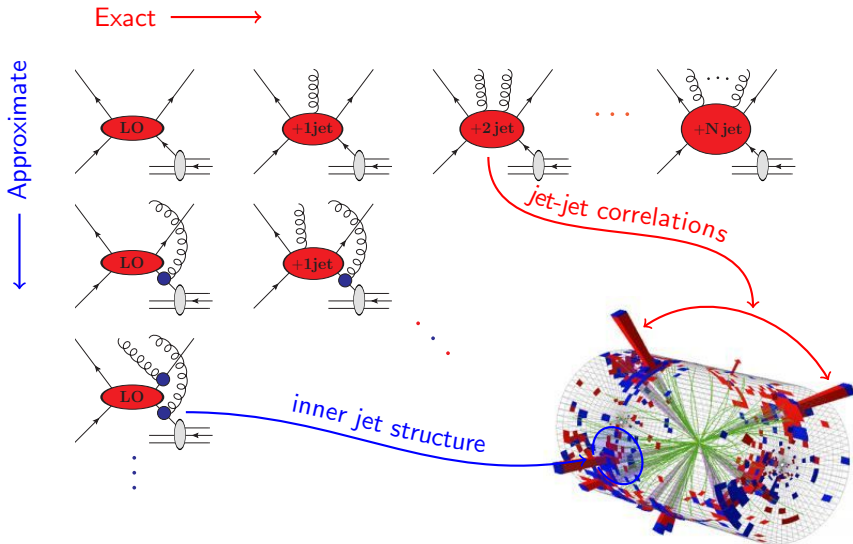


- A multi-scale problem

- $e^\pm q \rightarrow e^\pm q$ if $E_{T,B}^2 \lesssim Q^2$
 - $\gamma^* g \rightarrow jets$ if $Q^2 \lesssim E_{T,B}^2$

- What makes DIS different from $e^+e^- \rightarrow jj$ and $pp \rightarrow e^+e^-$ is that the virtuality of the exchanged photon tends to be close to zero

How to simulate it? Merging multiple LO calculations



Getting the physics right: Topology selection

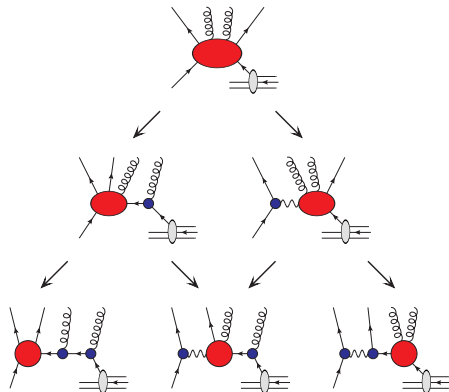
- QCD dynamics of the multi-jet final state must be reflected accurately when identifying a parton-shower branching tree

[Carli,Gehrmann,SH] arXiv:0912.3715

- $e^\pm q \rightarrow e^\pm q$ if $E_{T,B}^2 \lesssim Q^2$
- $\gamma^* g \rightarrow \text{jets}$ if $Q^2 \lesssim E_{T,B}^2$
- $qg \rightarrow \text{jets}$ if $Q^2 \ll E_{T,B}^2$

- Similar to taking direct and fragmentation component into account in hard photon production at hadron colliders

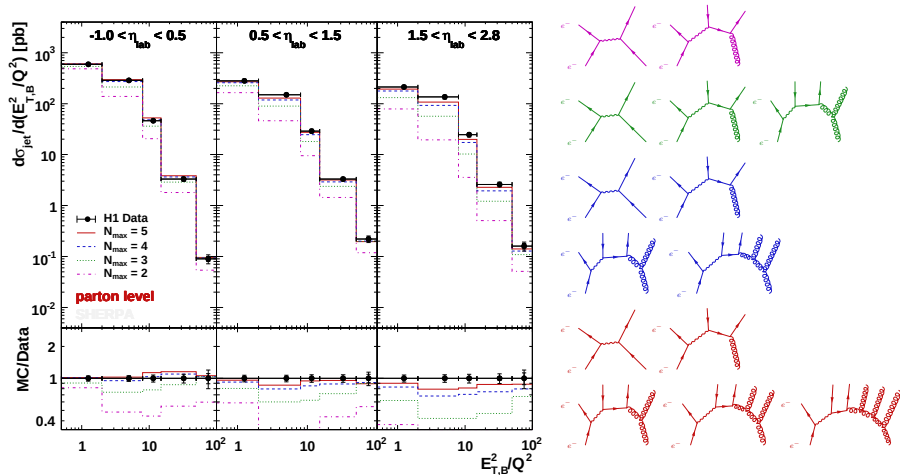
[Schumann,Siebert,SH] arXiv:0912.3501



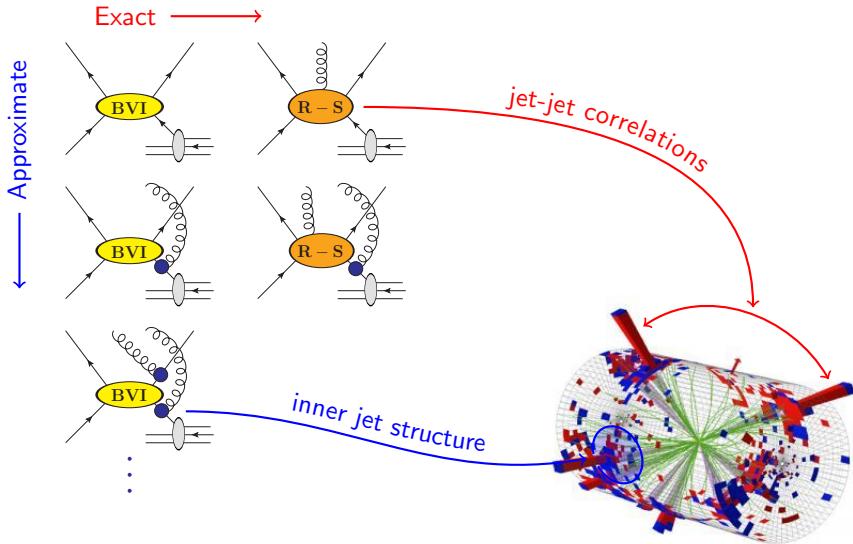
Comparison to HERA data

[Carli,Gehrmann,SH] arXiv:0912.3715

Variation of maximum matrix-element multiplicity, $N_{\max}$



How to simulate it? Matching NLO to parton showers



How to simulate it? Matching NLO to parton showers

Two major techniques to match NLO calculations and parton showers

MC@NLO

[Frixione,Webber] hep-ph/0204244

- ▶ Use parton-shower splitting kernel as infrared subtraction term
- ▶ Multiply LO event weight by Born-local K-factor including integrated subtraction term and virtual corrections
- ▶ Add hard remainder function consisting of subtracted real-emission correction

POWHEG

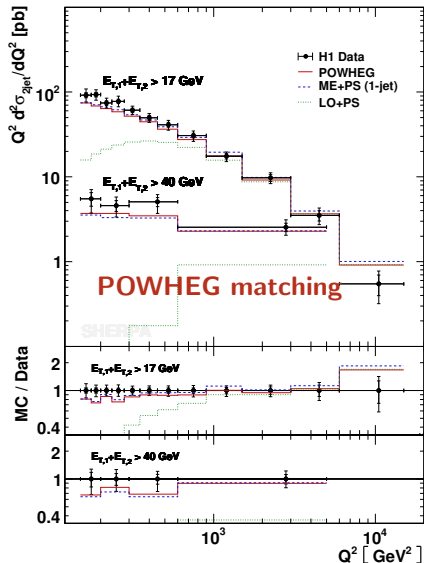
[Nason] hep-ph/0409146

- ▶ Use matrix-element corrections to replace parton-shower splitting kernel by full real-emission matrix element in first shower branching
- ▶ Multiply LO event weight by Born-local NLO K-factor (integrated over real corrections that can be mapped to Born according to parton-shower kinematics)

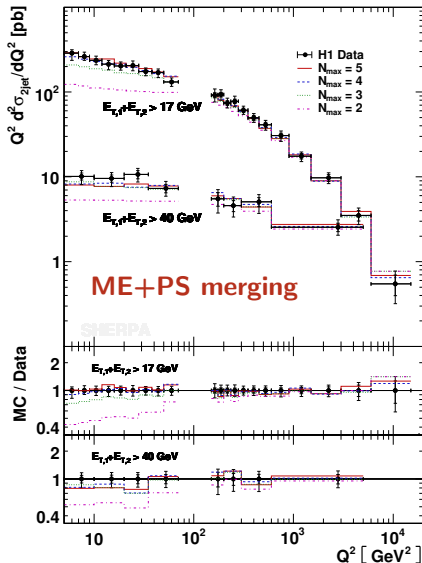
Both cases: Beware of sub-leading color terms and spin correlations!

Matching vs Merging: Which one is right for your purpose?

[Krauss,Schönherr,Siebert,SH] arXiv:1008.5399



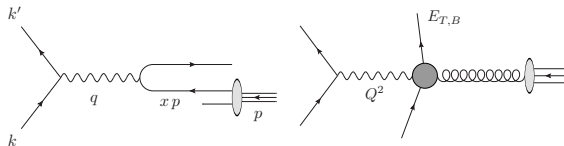
[Carli,Gehrmann,SH] arXiv:0912.3715



How to simulate it? Matching NNLO to parton showers

[Kuttimalai,Li,SH] arXiv:1809.04192

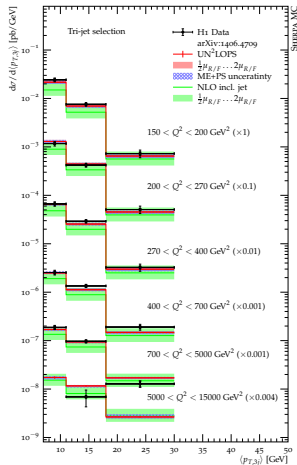
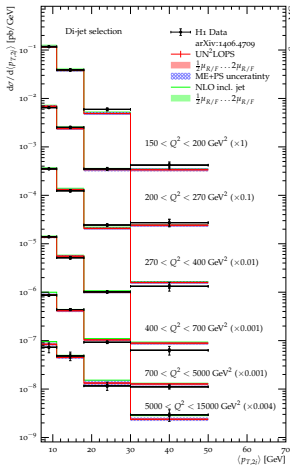
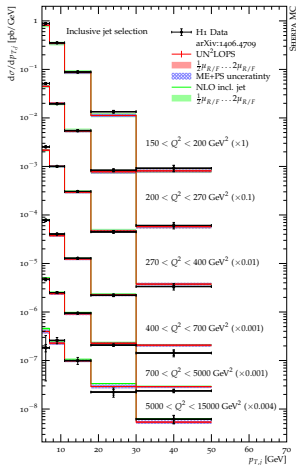
- ▶ Relatively straightforward to compute inclusive DIS at NNLO QCD
[Zijlstra,vanNeerven] NPB383(1992)525, PLB297(1992)377 [Moch,Vermaseren,Vogt] hep-ph/0504242
- ▶ Combined with Projection-to-Born method $\rightarrow$ fully differential NNLO
- ▶ UN²LOPS matching to parton shower for particle-level simulations
[Lönnblad,Prestel] arXiv:1211.7278, [Li,Prestel,SH] arXiv:1405.3607
- ▶ Scale choice appropriate for simultaneous description of inclusive DIS and inclusive jet / di-jet / tri-jet production $\rightarrow \mu_{R/F}^2 = (Q^2 + (H_T/2)^2)/2$



- ▶ Good agreement with H1 measurements in both high- Q^2 and low- Q^2 region [Andreev et al.] arXiv:1406.4709, arXiv:1611.03421

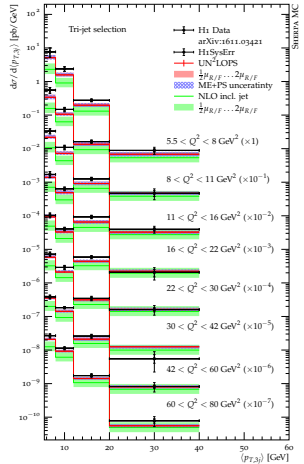
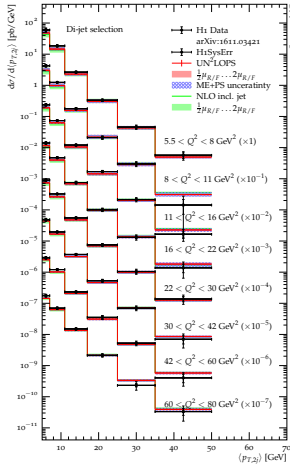
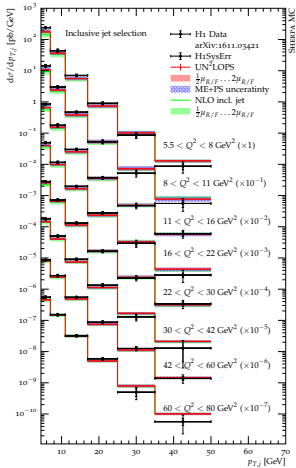
NNLO particle-level simulation vs. H1 high- Q^2 data

[Kuttimalai, Li, SH] arXiv:1809.04192



NNLO particle-level simulation vs. H1 low- Q^2 data

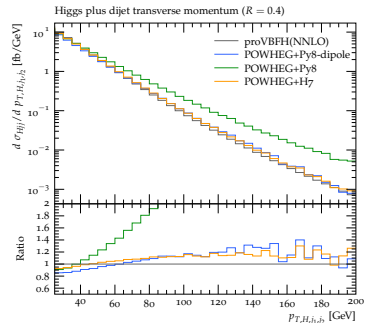
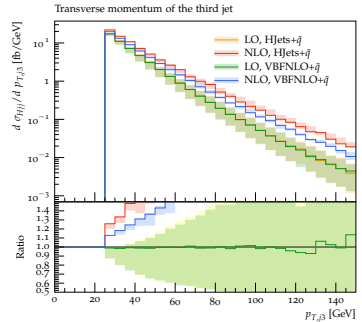
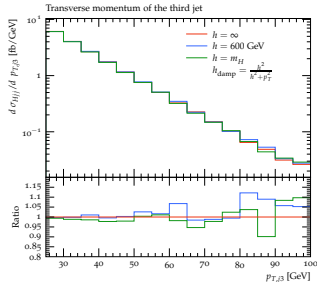
[Kuttimalai, Li, SH] arXiv:1809.04192



Where do we stand? N⁽²⁾LO / MC comparison in VBF

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

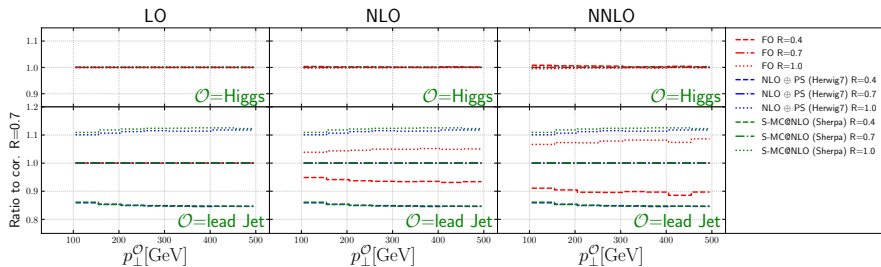
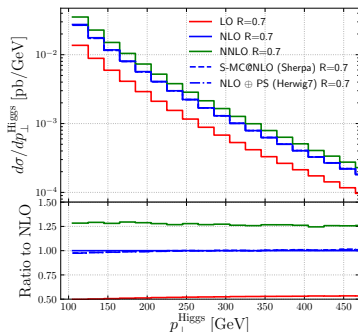
- Comparison between common tools Herwig/HJets, POWHEG/Pythia, and fixed-order NNLO
- Uncertainties of order 10% for more inclusive observables, order 20% for observables sensitive to radiative effects
- VBF process quite insensitive to form of Sudakov in POWHEG-BOX → little impact of hdamp parameter



Where do we stand? N⁽²⁾LO / MC comparison in $gg \rightarrow H_j$

[Bellm et al.] arXiv:1903.12563

- Good agreement between MC@NLO (Herwig / Sherpa) and fixed-order pQCD for inclusive observables in $pp \rightarrow H_j$
- 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 $\rightarrow$ alternative prescription needed, e.g. [Dasgupta,Dreyer,Salam,Soyez] arXiv:1602.01110



Current developments

► **Hard interaction**

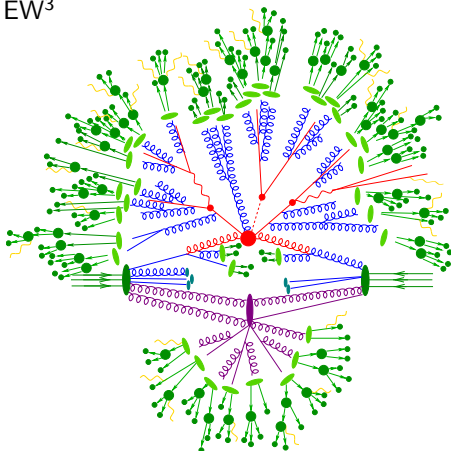
Extension of capabilities at NLO EW³
EW Sudakov resummation

► **Radiative corrections**

Matching at NLO QCD $\oplus/\otimes$ EW
Extension of parton showers to
NLO, NLL, NLC and beyond

► **Hadronization & Decays**

Hadronization at finite N_c
Dense QCD environments
Collective effects

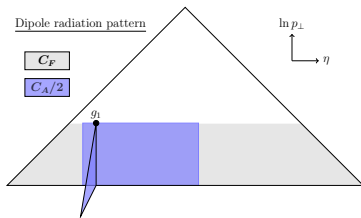
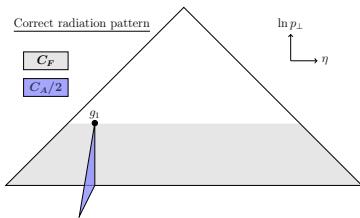
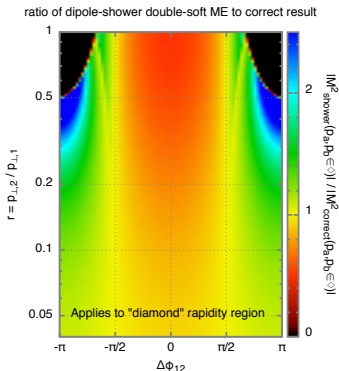


³via interfaces to 1-loop generators

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



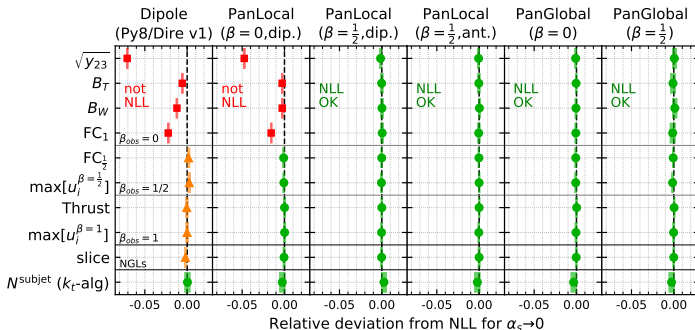
Parton showers beyond LL accuracy

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

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

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

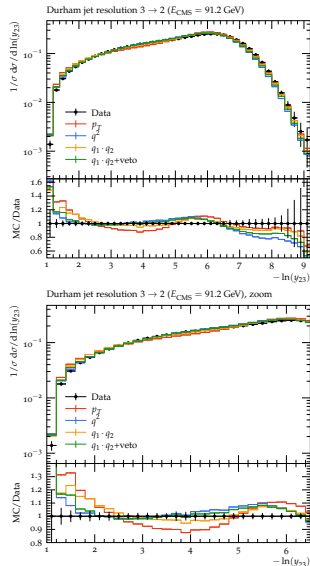
- Three different recoil schemes lead to NLL result if β chosen appropriately: Local dipole, local antenna, and global antenna
- First provably NLL correct parton shower for $e^+e^- \rightarrow \text{hadrons}$



Parton showers beyond LL accuracy

[Bewick,Ferrario-Ravasio,Richardson,Seymour] arXiv:1904.11866

- Recoil schemes affect logarithmic accuracy but impact also phase-space coverage
- In context of angular ordered Herwig 7 (NLL accurate for global observables)
 - q_T preserving scheme:
 - Maintains logarithmic accuracy
 - Overpopulates hard region
 - q^2 preserving scheme:
 - Breaks logarithmic accuracy
 - Good description of hard region
 - Dot product preserving scheme (new):
 - Maintains logarithmic accuracy
 - Good description of hard radiation



Towards parton showers at NLO

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

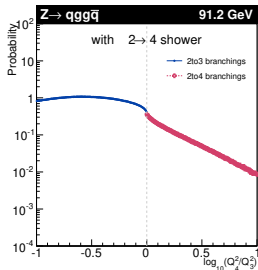
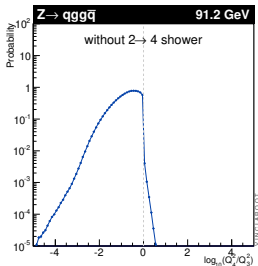
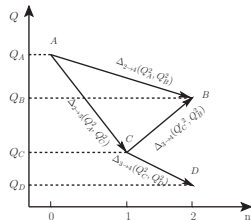
$$\begin{aligned}
 D_{ji}^{(0)}(z, \mu) &= \delta_{ij} \delta(1-z) & \leftrightarrow & \quad \text{[Diagram: Circle with incoming lines, outgoing line } j \text{ with momentum } z \text{]} / \text{[Diagram: Circle with incoming lines, outgoing line } i \text{ with momentum } 1 \text{]} \\
 D_{ji}^{(1)}(z, \mu) &= -\frac{1}{\epsilon} P_{ji}^{(0)}(z) & \leftrightarrow & \quad \text{[Diagram: Circle with incoming lines, outgoing line } i \text{ with momentum } z \text{ and a gluon emission from } i \text{]} / \text{[Diagram: Circle with incoming lines, outgoing line } i \text{ with momentum } 1 \text{]} \\
 D_{ji}^{(2)}(z, \mu) &= -\frac{1}{2\epsilon} P_{ji}^{(1)}(z) + \frac{\beta_0}{4\epsilon^2} P_{ji}^{(0)}(z) + \frac{1}{2\epsilon^2} \int_z^1 \frac{dx}{x} P_{jk}^{(0)}(x) P_{ki}^{(0)}(z/x) \\
 &\leftrightarrow \left(\text{[Diagram: Circle with incoming lines, outgoing line } i \text{ with momentum } z \text{ and a gluon emission from } i \text{]} + \text{[Diagram: Circle with incoming lines, outgoing line } i \text{ with momentum } z \text{ and a gluon emission from } i \text{]} \right) / \text{[Diagram: Circle with incoming lines, outgoing line } i \text{ with momentum } 1 \text{]}
 \end{aligned}$$

- 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

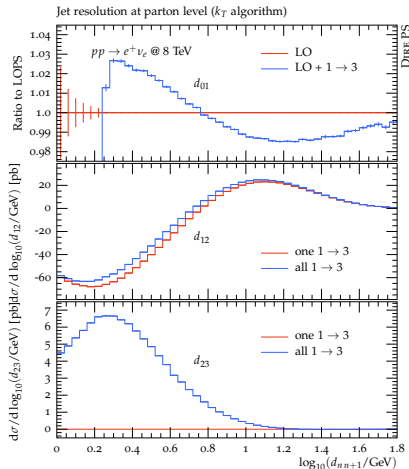


Towards parton showers at NLO

- 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)

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

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



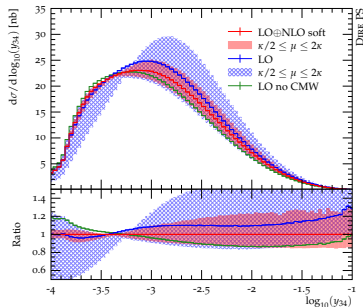
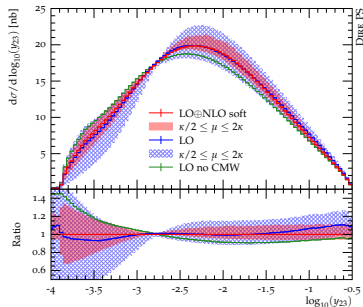
Towards parton showers at NLO

[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

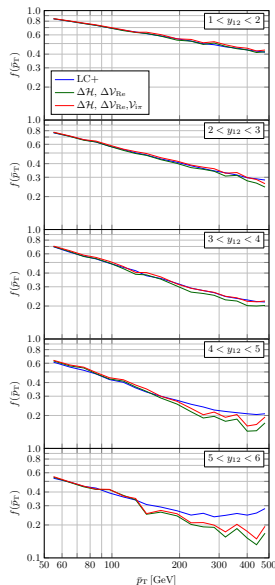


Parton showers beyond LC accuracy

[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



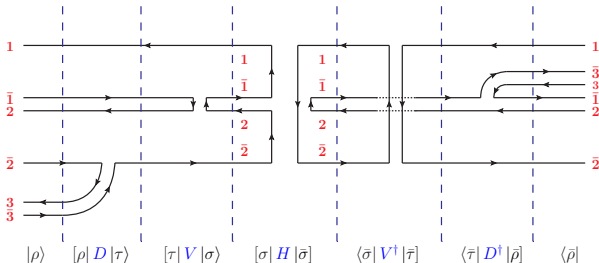
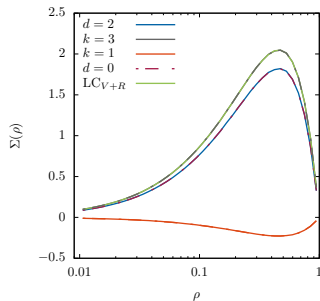
Parton showers beyond LC accuracy

[DeAngelis,Forshaw,Plätzer] arXiv:2007.09648

[Forshaw,Holguin,Plätzer] arXiv:1905.08686

- 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 $n = 1$

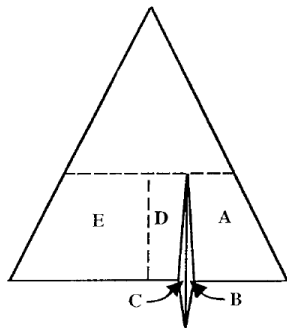


Parton showers beyond LC accuracy

[Gustafsson] Nucl.Phys.B392(1993)251-280

[Hamilton,Medves,Salam,Scyboz,Soyez] arXiv:2011.10054

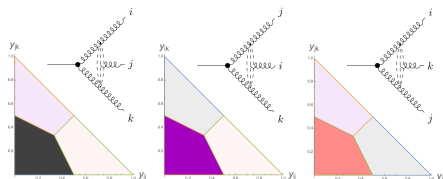
- ▶ Different parts of phase space for coherent emission off a $q\bar{q}g$ system can be associated with individual hard partons (jets)
- ▶ Best visualized in Lund plane
 - ▶ Region A: q jet
 - ▶ Region B&C: g jet
 - ▶ Region E: $\bar{q}$ jet
- ▶ Region D: Coherent emission off $\bar{q}g$ system
Color charge is that of “mother” $\bar{q}$ -jet $\rightarrow C_F$
- ▶ Extension to all orders: Emissions in Lund “back-plane” have color factor C_F , even if emitting large- N_c dipole is gluon pair



Sector showers

[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

Deep Inelastic Scattering

- ▶ A precision laboratory for validating and calibrating MCs
- ▶ Simulations possible up to NNLO QCD precision
- ▶ NLO (merged) simulations available in all major generators
- ▶ Incorporation of QED/EW corrections one of next milestones

More generally

- ▶ Good agreement between different MC generators when using similar setups & assumptions (not trivial!)
- ▶ 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

Thank you for your attention!

Availability of DIS simulations

► Herwig

- Matching fully automated [Gieseke,Plätzer] arXiv:1109.6256
- External 1-loop providers & builtin loop library
- Merging in modified unitarized approach [Plätzer] arXiv:1211.5467, [Bellm,Gieseke,Plätzer] arXiv:1705.06700
- QED & mixed higher-order corrections work in progress

► Pythia

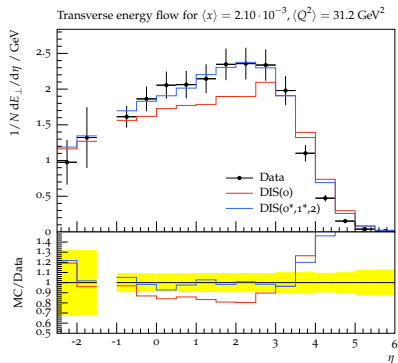
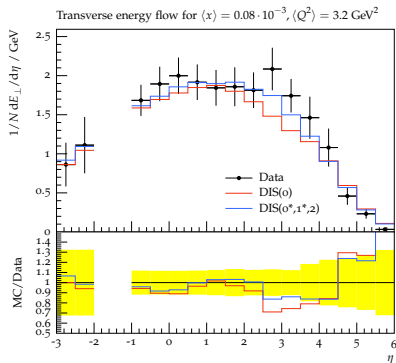
- New parton shower Dire [Prestel,SH] arXiv:1506.05057
- Unitarized merging under development [Prestel,Lönnblad] arXiv:1211.4827
- Matching via interface to POWHEG / MC@NLO

► Sherpa

- Matching fully automated [Krauss,Schönherr,Siebert,SH] arXiv:1008.5399, arXiv:1111.1220
- External 1-loop providers & builtin loop library
- Merging in non-unitarized approach [Krauss,Schönherr,Siebert,SH] arXiv:1207.5030
- NNLO matching [Kuttimalai,Li,SH] arXiv:1809.04192

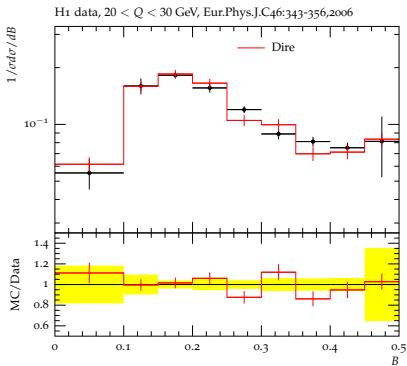
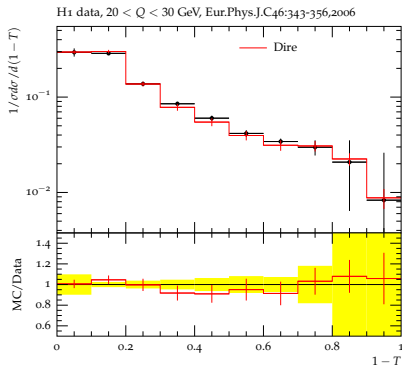
Performance examples – Herwig

- NLO Merged calculation vs data from hep-ex/9907027



Performance examples – Pythia

- Parton-shower calculation vs data from [hep-ex/0512014](#)



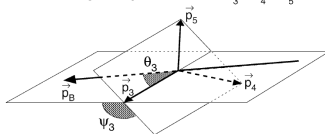
Performance examples – Sherpa

[Carli,Gehrmann,SH] arXiv:0912.3715

three-jet center-of-mass frame:

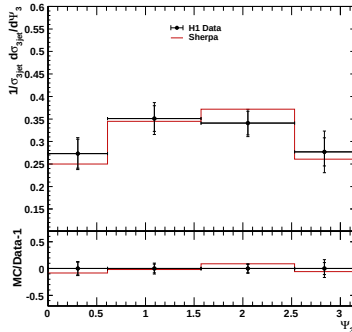
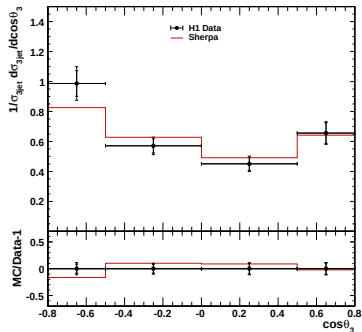
$1 + 2 \rightarrow 3 + 4 + 5$

$E_3 > E_4 > E_5$



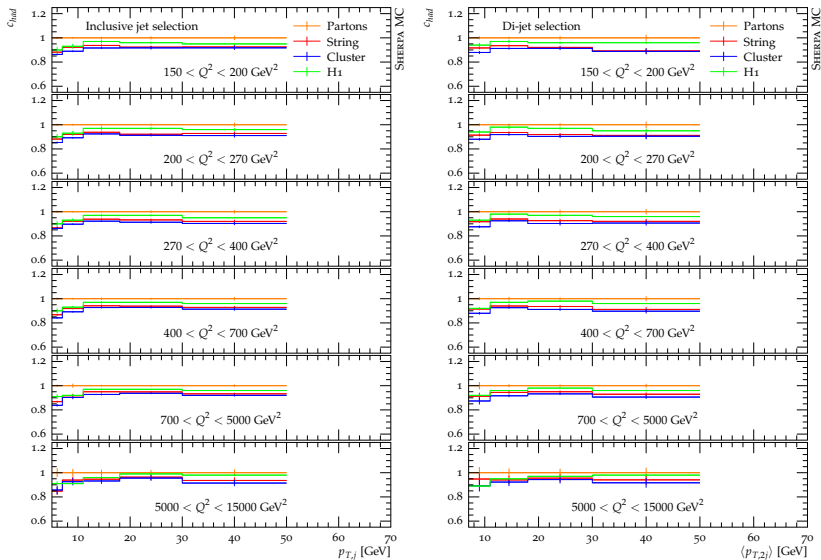
$\cos \theta_3 \quad Q^2 > 150 \text{ GeV}^2$

$\Psi_3 \quad Q^2 > 150 \text{ GeV}^2$



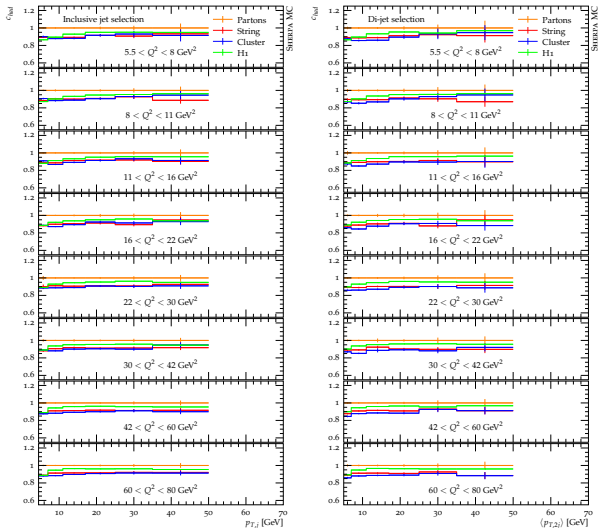
Hadronization corrections at high Q^2

[Kuttimalai,Li,SH] arXiv:1809.04192



Hadronization corrections at low Q^2

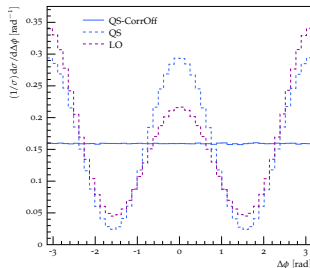
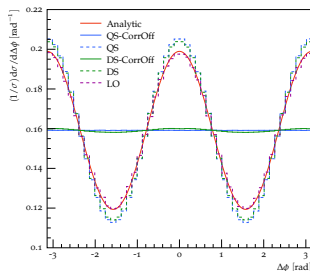
[Kuttimalai,Li,SH] arXiv:1809.04192



Spin correlations in decays and showers

- Spin-correlation algorithms known since '80s [Collins] NPB304(1988)794, [Knowles] CPC58(1990)271, [Richardson] hep-ph/0110108
- Decay correlations in $\sim$ all generators [Gigg,Richardson] hep-ph/0703199 [Artoisenet, Frederix,Mattelaer,Rietkerk] arXiv:1212.3460 [Kuttimalai,Schumann,Siebert,SH] arXiv:1412.6478
- Spin-dependent parton showers Herwig [Richardson,Webster] arXiv:1807.01955 Vincia [Fischer,Lifson,Skands] arXiv:1708.01736

[Richardson,Webster] arXiv:1807.01955



Improved NLO matching

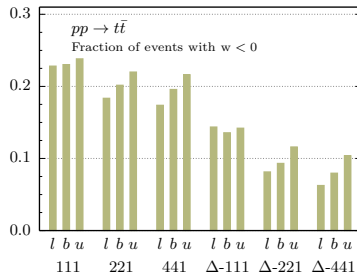
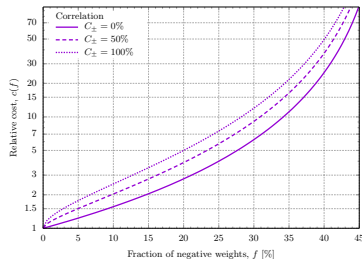
[Frederix,Frixione,Prestel,Torrielli] arXiv:2002.12716

- 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

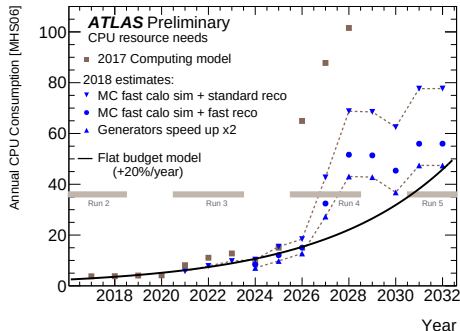
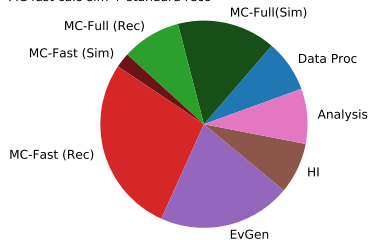


Computing challenges

[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)

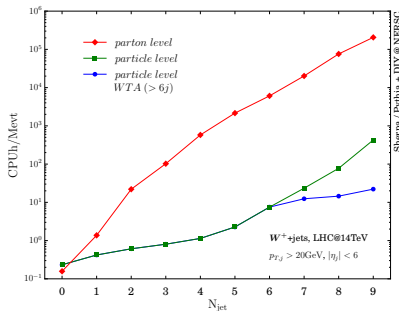
ATLAS Preliminary. 2028 CPU resource needs
MC fast calo sim + standard reco



[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 ~ 2048 cores
- Event generation step scales (strong & weak) up to ~ 2048 cores
- Performance limited by number of events being processed per rank (Average timing can only be expected if statistics is large enough)

