

# Precision simulations of light and heavy jets

Stefan Höche

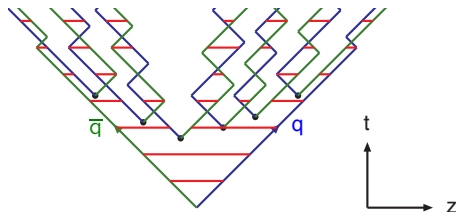
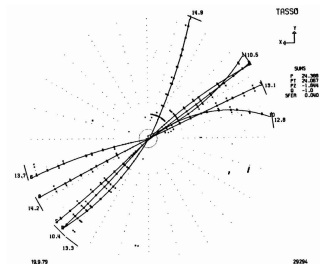
Fermi National Accelerator Laboratory

Theory Seminar

Jagiellonian University in Krakow, 04/05/2024

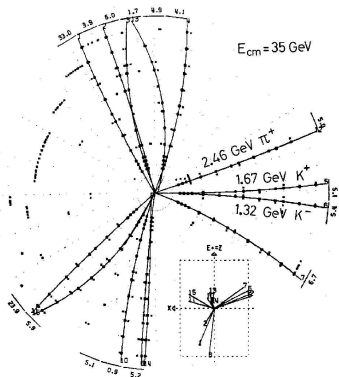
# Collider events before PETRA

[Andersson,Gustafson,Ingelman,Sjöstrand] Phys.Rept.97(1983)31



- Lund string model: QCD flux tube like a rubber band that is pulled apart → breaks into pieces, generating many smaller flux tubes.
- Creates two collimated sprays of hadrons → 2-jet events
- Complete description of the physics at low-energy  $e^+e^-$ -colliders

# The gluon changes everything



22.9.80

Neutrino '79: Event 13177 makes history

Image credit: DESY, P. Duinker

# The gluon changes everything

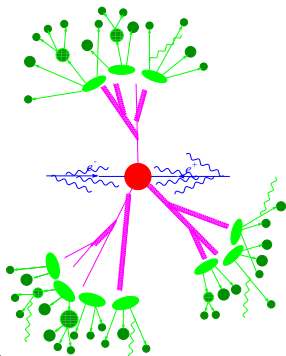
[Marchesini,Webber] Nucl.Phys.B238(1984)1, [Webber] Nucl.Phys.B238(1984)492  
[Andersson,Gustafson,Ingelman,Sjöstrand] Phys.Rept.97(1983)31

- Short distance interactions
  - Signal process
  - QCD radiative corrections
- Long-distance interactions
  - Hadronization
  - Particle decays

## Divide and Conquer

- Quantity of interest: Interaction rate
- Convolution of short & long distance physics

$$\sigma_{ee \rightarrow h+X} = \sum_{i \in \{q,g\}} \int dx \underbrace{\hat{\sigma}_{ee \rightarrow i+X}(x, \mu_F^2)}_{\text{short distance}} \underbrace{D_i^{(h)}(x, \mu_F^2)}_{\text{long distance}}$$



# Forty years and many discoveries later ...

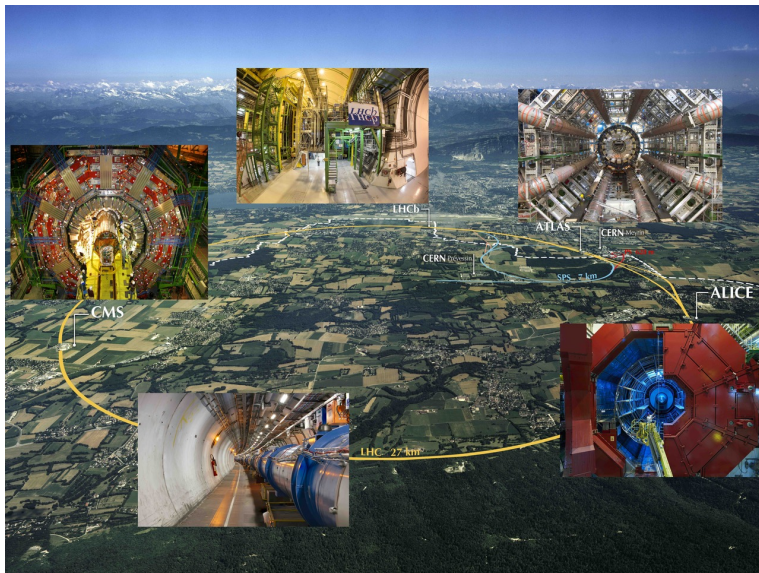
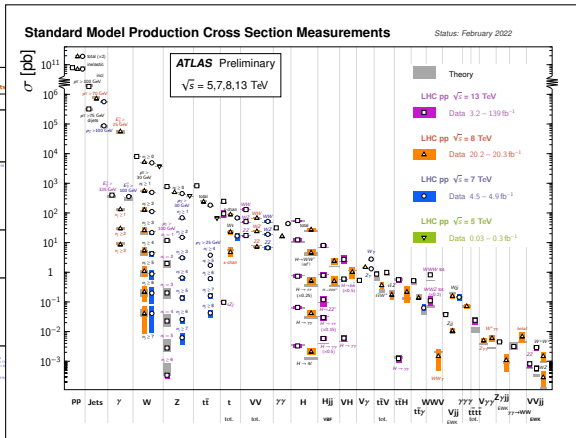
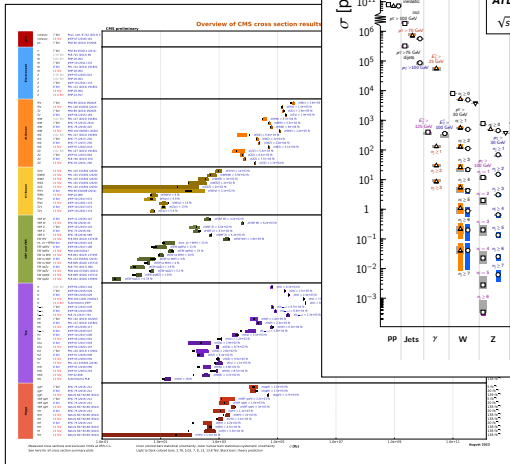


Image credit: CERN

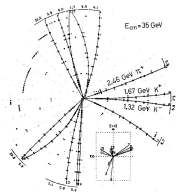
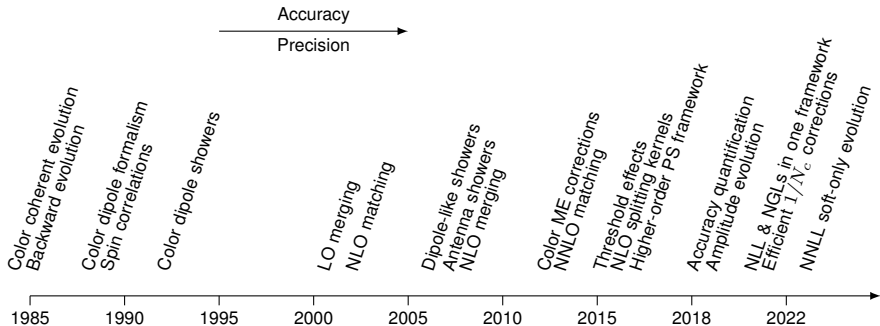
# ... it's all about jets



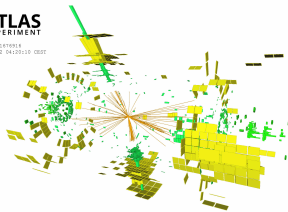
[ATLAS] <https://twiki.cern.ch/twiki/bin/view/AtlasPublic/StandardModelPublicResults>

[CMS] <https://twiki.cern.ch/twiki/bin/view/CMSPublic/PhysicsResultsCombined>

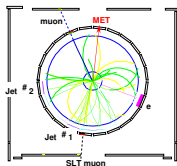
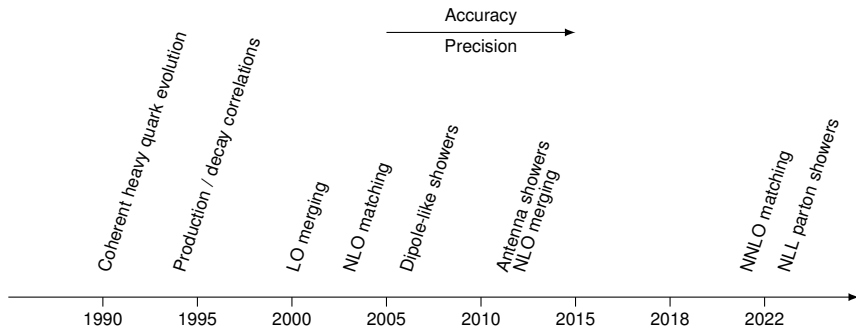
# So we need to simulate jets ...



$\sqrt{s} \times 500$   
 $e^+e^-$  vs.  $pp$

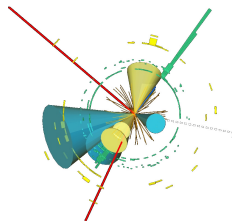


# ... sometimes fat jets ...



$$\sqrt{s} \times 7$$

$p\bar{p}$  vs.  $pp$

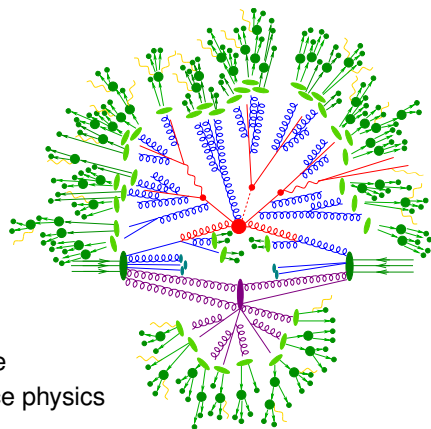




# ... but always many jets

[Buckley et al.] arXiv:1101.2599  
[Campbell et al.] arXiv:2203.11110

- Short distance interactions
  - Signal process
  - Radiative corrections
- Long-distance interactions
  - Hadronization
  - Particle decays



## Divide and Conquer

- Quantity of interest: Interaction rate
- Convolution of short & long distance physics

$$\sigma_{p_1 p_2 \rightarrow X} = \sum_{i,j \in \{q,g\}} \int dx_1 dx_2 \underbrace{f_{p_1,i}(x_1, \mu_F^2) f_{p_2,j}(x_2, \mu_F^2)}_{\text{long distance}} \underbrace{\hat{\sigma}_{ij \rightarrow X}(x_1 x_2, \mu_F^2)}_{\text{short distance}}$$

# The connection to pQCD theory

- $\hat{\sigma}_{ij \rightarrow n}(\mu_F^2) \rightarrow$  Collinearly factorized fixed-order result at N<sup>x</sup>LO

Implemented in fully differential form to be maximally useful

Tree level:  $d\Phi_n B_n$

- Automated ME generators + phase-space integrators

1-Loop level:  $d\Phi_n \left( B_n + V_n + \sum C + \sum I_n \right) + d\Phi_{n+1} \left( R_n - \sum S_n \right)$

- Automated loop ME generators + integral libraries + IR subtraction

2-Loop level: It depends ...

- Individual solutions based on SCET,  $q_T$  subtraction, P2B

- $f_i(x, \mu_F^2) \rightarrow$  Collinearly factorized PDF at N<sup>y</sup>LO

Evaluated at  $O(1\text{GeV}^2)$  and expanded into a series above  $1\text{GeV}^2$

$$\text{DGLAP: } \frac{dx x f_a(x, t)}{d \ln t} = \sum_{b=q,g} \int_0^1 d\tau \int_0^1 dz \frac{\alpha_s}{2\pi} [z P_{ab}(z)]_+ \tau f_b(\tau, t) \delta(x - \tau z)$$

- Parton showers, dipole showers, antenna showers, ...

$$\text{Matching: } d\Phi_n \frac{S_n}{B_n} \leftrightarrow \frac{dt}{t} dz \frac{\alpha_s}{2\pi} P_{ab}(z)$$

- MC@NLO, POWHEG, Geneva, MINNLO<sub>PS</sub>, ...

# Simulation of QCD dipole radiation

## Approaches, problems & solutions

# Semi-classical radiation pattern

[Marchesini,Webber] NPB310(1988)461

- Soft gluon radiator can be written in terms of energies and angles

$$J_\mu J^\mu \rightarrow \frac{p_i p_k}{(p_i p_j)(p_j p_k)} = \frac{W_{ik,j}}{E_j^2}$$

Angular “radiator” function

$$W_{ik,j} = \frac{1 - \cos \theta_{ik}}{(1 - \cos \theta_{ij})(1 - \cos \theta_{jk})}$$

- Divergent as  $\theta_{ij} \rightarrow 0$  and as  $\theta_{jk} \rightarrow 0$

→ Expose individual collinear singularities using  $W_{ik,j} = \tilde{W}_{ik,j}^i + \tilde{W}_{ik,j}^k$

$$\tilde{W}_{ik,j}^i = \frac{1}{2} \left[ \frac{1 - \cos \theta_{ik}}{(1 - \cos \theta_{ij})(1 - \cos \theta_{kj})} + \frac{1}{1 - \cos \theta_{ij}} - \frac{1}{1 - \cos \theta_{kj}} \right]$$

- Divergent as  $\theta_{ij} \rightarrow 0$ , but regular as  $\theta_{kj} \rightarrow 0$
- Convenient properties upon integration over azimuthal angle

# Semi-classical radiation pattern

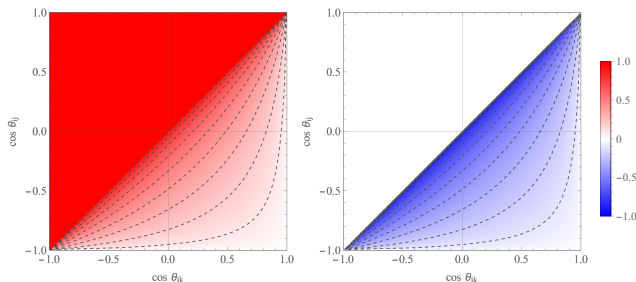
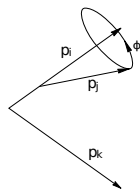
- Work in a frame where direction of  $\vec{p}_i$  aligned with  $z$ -axis

$$\cos \theta_{kj} = \cos \theta_k^i \cos \theta_j^i + \sin \theta_k^i \sin \theta_j^i \cos \phi_{kj}^i$$

- Integration over  $\phi_j$  yields

$$\frac{1}{2\pi} \int_0^{2\pi} d\phi_{kj}^i \tilde{W}_{ik,j}^i = \frac{1}{1 - \cos \theta_j^i} \times \begin{cases} 1 & \text{if } \theta_j^i < \theta_k^i \\ 0 & \text{else} \end{cases}$$

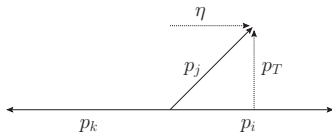
- On average, no radiation outside cone defined by parent dipole
- Differential radiation pattern more intricate:  
Positive & negative contributions outside cone sum to zero



# Dual description and the Lund plane

[Gustafson] PLB175(1986)453

- Compute everything in center-of-mass frame of fast partons



- Simple expressions for transverse momentum and rapidity

$$p_T^2 = \frac{2(p_i p_j)(p_k p_j)}{p_i p_k}, \quad \eta = \frac{1}{2} \ln \frac{p_i p_j}{p_k p_j}$$

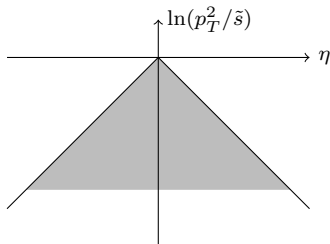
- In momentum conserving parton branching  $(\tilde{p}_i, \tilde{p}_k) \rightarrow (p_i, p_k, p_j)$

$$-\ln \tilde{s}_{ik}/p_T^2 \leq 2\eta \leq \ln \tilde{s}_{ik}/p_T^2$$

- Differential phase-space element  $\propto dp_T^2 d\eta$

- Visualized in Lund plane

- Phase space bounded by diagonals
- Single-emission semi-classical radiation probability a constant



# Angular ordered parton showers

[Marchesini,Webber] NPB238(1984)1, ...

## ■ Differential radiation probability

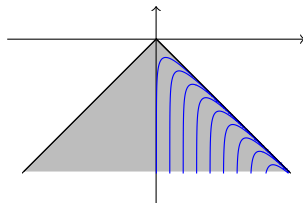
$$d\mathcal{P} = d\Phi_{+1} |M|^2 \approx \frac{d\tilde{q}^2}{\tilde{q}^2} dz \frac{\alpha_s}{2\pi} P_{i\tilde{j}i}(z)$$

- Ordering parameter  $\tilde{q}^2 = \frac{2p_i p_j}{z(1-z)} \approx 4E_{ij}^2 \sin^2 \frac{\theta_{ij}}{2}$

- Splitting variable  $z = \frac{1 + \cos \theta_{ik}}{2} = \frac{p_i p_k}{(p_i + p_j) p_k}$

## ■ Lund plane filled from center to edges

- Random walk in  $p_T^2$
- Color factors correct for observables insensitive to azimuthal correlations
- Small dead zone at  $\ln(p_T^2/\bar{s}) \approx 0$



- Usually disfavored due to dead zones  
Not suitable to resum non-global logarithms

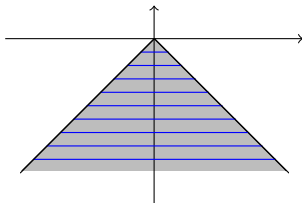
# Dipole showers

[Gustafson, Pettersson] NPB306(1988)746, ...

- Differential radiation probability for the dipole

$$d\mathcal{P} = d\Phi_{+1} |M|^2 \approx \frac{dp_T^2}{p_T^2} d\eta \frac{\alpha_s}{2\pi} \tilde{P}_{\tilde{\gamma}}(z)$$

- Ordering parameter  $p_T^2$
- Splitting variable  $z = 1 - \frac{s_{ij}}{s - s_{ij}} e^{-2\eta}$
- Lund plane filled from top to bottom
  - Random walk in  $\eta$
  - Color factors in CFFE approximation
  - Pairs of partons evolve simultaneously
  - No dead zones
- Solves problem of dead zones  
Known issues with color coherence

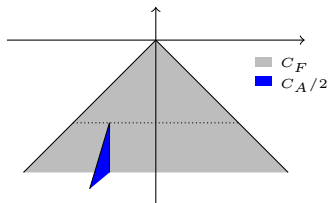




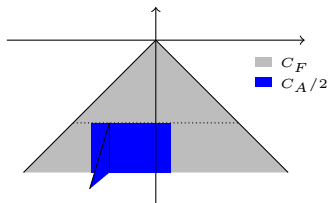
# Problems with average color charges

[Gustafsson] NPB392(1993)251

- In angular ordered showers angles are measured in the event center-of-mass frame  
→ coherence effects modeled by angular ordering variable agree on average with matrix element



- In dipole-like showers angles effectively measured in center-of-mass frame of emitting color dipole  
→ angular coherence not reflected by setting average QCD charge



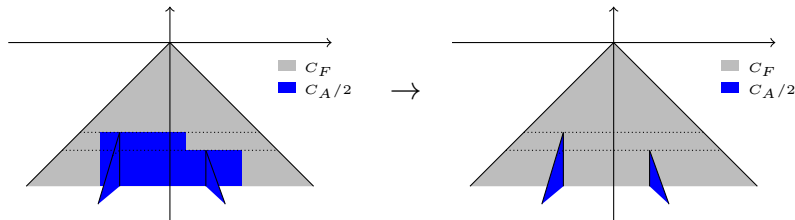
- Emission off “back plane” in Lund diagram should be associated with  $C_F$ , but is partly associated with  $C_A/2$  in dipole showers
- All-orders problem that appears first in 2-gluon emission case

# Solutions for average color charges

[Gustafsson] NPB392(1993)251

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

- Analyze rapidity of gluon emission in event center-of-mass frame
- Sectorize phase space and assign gluon to closest parton  
→ choose corresponding color charge for evolution
- Same technology for higher number of emissions



- Starting with 4 emissions, there be “color monsters”

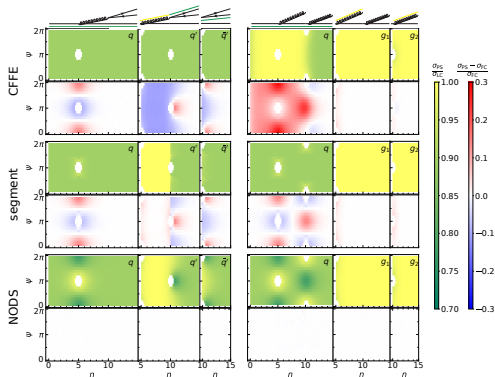
[Dokshitzer,Troian,Khoze] SJNP47(1988)881, YF47(1988)1384

- Quartic Casimir operators (easy)
- Non-factorizable contributions (hard)

# Solutions for average color charges

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

- Can include double-soft corrections via reweighting [Giele,Kosower,Skands] arXiv:1102.2126
- Algorithm scales as  $N^2$  but can be simplified while retaining formal accuracy
- Implementation as nested corrections in rapidity segments of parent dipole
- Excellent agreement with full matrix element
- Good agreement with full-color evolution [Hatta,Ueda] arXiv:1304.6930



# Problems with momentum mapping

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

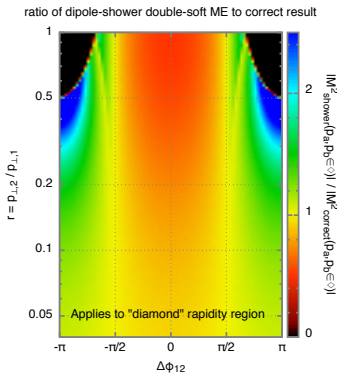
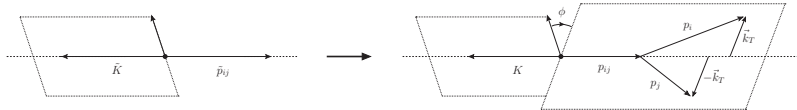
- Subtle problems in standard dipole-like momentum mapping

$$p_k^\mu = \left(1 - \frac{p_{ij}^2}{2\tilde{p}_{ij}\tilde{p}_k}\right) \tilde{p}_k^\mu$$

$$p_i^\mu = \tilde{z}\tilde{p}_{ij}^\mu + (1 - \tilde{z})\frac{p_{ij}^2}{2\tilde{p}_{ij}\tilde{p}_k}\tilde{p}_k^\mu + k_\perp^\mu$$

$$p_j^\mu = (1 - \tilde{z})\tilde{p}_{ij}^\mu + \tilde{z}\frac{p_{ij}^2}{2\tilde{p}_{ij}\tilde{p}_k}\tilde{p}_k^\mu - k_\perp^\mu$$

- Induces angular correlations across multiple emissions
- Spoils agreement w/ analytic resummation



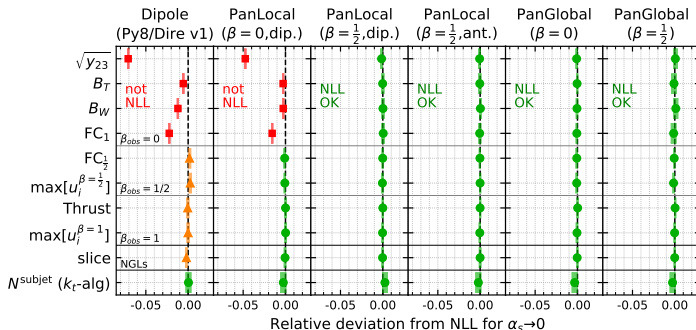
# Solutions for momentum mapping

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

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

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

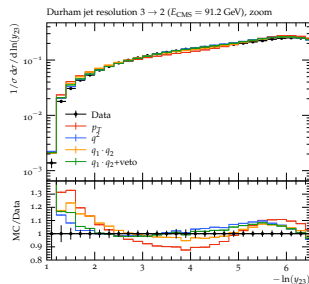
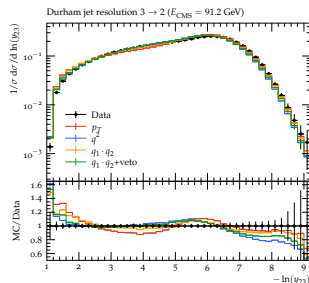
- Different recoil schemes can lead to NLL result if  $\beta$  chosen appropriately: Local dipole, local antenna, and global antenna
- NLL correct for global and non-global observables in  $e^+e^- \rightarrow \text{hadrons}$



# Solutions for momentum mapping

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

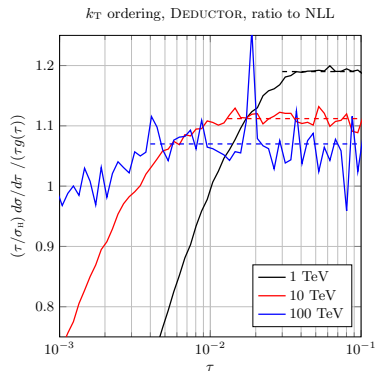
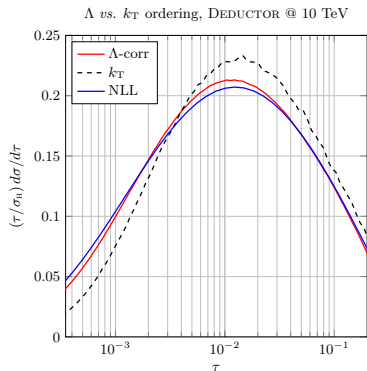
- Recoil schemes affect logarithmic accuracy but impact also phase-space coverage
- In context of angular ordered Herwig 7 (NLL accurate for global observables)
  - $q_T$  preserving scheme:
    - Maintains logarithmic accuracy
    - Overpopulates hard region
  - $q^2$  preserving scheme:
    - Breaks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



# Solutions for momentum mapping

[Nagy,Soper] arXiv:2011.04773

- Local transverse recoil, global longitudinal recoil
- Analytic proof of NLL correctness, based on kinematics in  $s \rightarrow \infty$  limit



**A new perspective on old ideas**

**Identified partons & azimuthal angle dependence**



# The semi-classical matrix element revisited

- Alternative to additive matching: partial fraction matrix element & match to collinear sectors [Ellis,Ross,Terrano] NPB178(1981)421, [Catani,Seymour] hep-ph/9605323

$$\frac{W_{ik,j}}{E_j^2} \rightarrow \frac{1}{p_i p_j} \frac{p_i p_k}{(p_i + p_k) p_j} + \frac{1}{p_k p_j} \frac{p_i p_k}{(p_i + p_k) p_j}$$

- Captures matrix element both in angular ordered and unordered region
  - Caveat: Oversampling difficult for certain kinematics maps
- Separate into energy & angle first [Herren,Krauss,Reichelt,Schönherr,SH] arXiv:2208.06057  
 Partial fraction angular radiator only:  $W_{ik,j} = \bar{W}_{ik,j}^i + \bar{W}_{ki,j}^k$

$$\bar{W}_{ik,j}^i = \frac{1 - \cos \theta_{ik}}{(1 - \cos \theta_{ij})(2 - \cos \theta_{ij} - \cos \theta_{kj})}$$

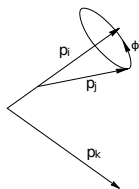
- Bounded by  $(1 - \cos \theta_{ij}) \bar{W}_{ik,j}^i < 2$
- Strictly positive

# The semi-classical matrix element revisited

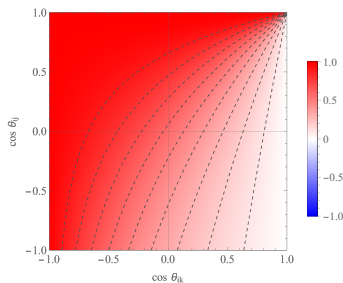
- Integration over  $\phi_j$  yields

$$\frac{1}{2\pi} \int_0^{2\pi} d\phi_{kj}^i \bar{W}_{ik,j}^i = \frac{1}{1 - \cos \theta_j^i} \frac{1}{\sqrt{(\bar{A}_{ij,k}^i)^2 - (\bar{B}_{ij,k}^i)^2}}$$

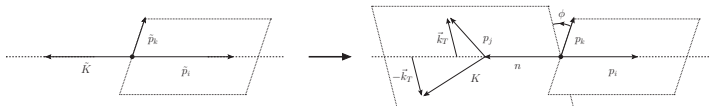
- Radiation across all of phase space
- Probabilistic radiation pattern



$$\bar{A}_{ij,k}^i = \frac{2 - \cos \theta_j^i (1 + \cos \theta_k^i)}{1 - \cos \theta_k^i}$$
$$\bar{B}_{ij,k}^i = \frac{\sqrt{(1 - \cos^2 \theta_j^i)(1 - \cos^2 \theta_k^i)}}{1 - \cos \theta_k^i}$$



# Kinematics mapping revisited



- In collinear limit, splitting kinematics defined by ( $n \rightarrow$  auxiliary vector)

$$p_i \xrightarrow{i||j} z \tilde{p}_i, \quad p_j \xrightarrow{i||j} (1-z) \tilde{p}_i \quad \text{where} \quad z = \frac{p_i n}{(p_i + p_j) n}$$

- Parametrization, using hard momentum  $\tilde{K}$

$$p_i = z \tilde{p}_i, \quad n = \tilde{K} + (1-z) \tilde{p}_i$$

- Using on-shell conditions & momentum conservation ( $\kappa = \tilde{K}^2 / (2\tilde{p}_i \tilde{K})$ )

$$p_j = (1-z) \tilde{p}_i + v(\tilde{K} - (1-z + 2\kappa) \tilde{p}_i) + k_{\perp}$$

$$K = \tilde{K} - v(\tilde{K} - (1-z + 2\kappa) \tilde{p}_i) - k_{\perp}$$

- Momenta in  $\tilde{K}$  Lorentz-boosted to new frame  $K$  [Catani,Seymour] hep-ph/9605323

$$p_l^{\mu} \rightarrow \Lambda_{\nu}^{\mu}(K, \tilde{K}) p_l^{\nu}, \quad \Lambda_{\nu}^{\mu}(K, \tilde{K}) = g_{\nu}^{\mu} - \frac{2(K + \tilde{K})^{\mu}(K + \tilde{K})_{\nu}}{(K + \tilde{K})^2} + \frac{2\tilde{K}^{\mu} K_{\nu}}{K^2}.$$

# Logarithmic accuracy – Analytic proof

- Logarithmic accuracy of parton shower can be quantified by comparing results to (semi-)analytic resummation e.g. [Banfi,Salam,Zanderighi] hep-ph/0407286
- Example: Thrust or  $FC_0$  in  $e^+e^- \rightarrow \text{hadrons}$
- Define a shower evolution variable  $\xi = k_T^2/(1-z)$
- Parton-shower one-emission probability for  $\xi > Q^2\tau$

$$R_{\text{PS}}(\tau) = 2 \int_{Q^2\tau}^{Q^2} \frac{d\xi}{\xi} \int_{z_{\min}}^{z_{\max}} dz \frac{\alpha_s(k_T^2)}{2\pi} C_F \left[ \frac{2}{1-z} - (1+z) \right] \Theta(\eta)$$

- Approximate to NLL accuracy

$$R_{\text{NLL}}(\tau) = 2 \int_{Q^2\tau}^{Q^2} \frac{d\xi}{\xi} \left[ \int_0^1 dz \frac{\alpha_s(k_T^2)}{2\pi} \frac{2C_F}{1-z} \Theta(\eta) - \frac{\alpha_s(\xi)}{\pi} C_F B_q \right]$$

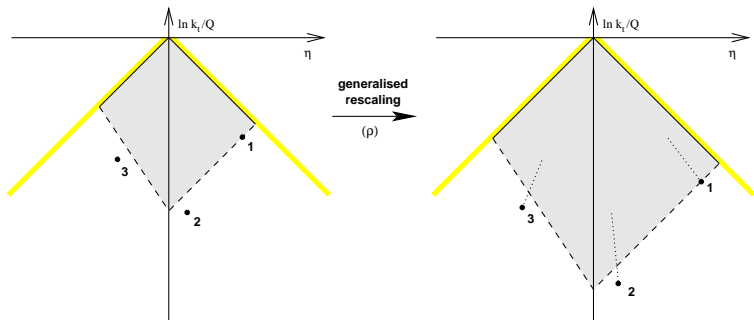
# Logarithmic accuracy – Analytic proof

- Cumulative cross section  $\Sigma(\tau) = e^{-R(\tau)} \mathcal{F}(\tau)$  obtained from all-orders resummed result by Taylor expansion of virtual corrections in cutoff  $\varepsilon$

$$\mathcal{F}(\tau) = \int d^3 k_1 |M(k_1)|^2 e^{-R' \ln \frac{\tau}{\varepsilon v_1}} \sum_{m=0}^{\infty} \frac{1}{m!} \left( \prod_{i=2}^{m+1} \int_{\varepsilon v_1}^{v_1} d^3 k_i |M(k_i)|^2 \right) \times \Theta(\tau - V(\{p\}, k_1, \dots, k_n))$$

- $\mathcal{F}(\tau)$  is pure NLL & accounts for (correlated) multiple-emission effects
- In order to make  $\mathcal{F}(\tau)$  calculable, make the following assumptions
  - Observable is recursively infrared and collinear safe
  - Hold  $\alpha_s(Q^2) \ln \tau$  fixed, while taking limit  $\tau \rightarrow 0$ 
    - Can factorize integrals and neglect kinematic edge effects
- Can be interpreted as  $\alpha_s \rightarrow 0$  or  $s \rightarrow \infty$  limit**

# Logarithmic accuracy – Analytic proof



- $\alpha_s \rightarrow 0 / s \rightarrow \infty$  limit taken by similarity transformation of Lund plane
- Can be parametrized in terms of scaling parameter  $\rho$

$$k_{t,l} \rightarrow k'_{t,l} = k_{t,l} \rho^{(1-\xi_l)/a + \xi_l/(a+b)}$$

$$\eta_l \rightarrow \eta'_l = \eta - \xi_l \frac{\ln \rho}{a+b}, \quad \text{where} \quad \xi = \frac{\eta}{\eta_{\max}}$$

observable parametrization at one-emission level:  $v = (k_t^2/Q^2)^a \exp(-b\eta)$

- NLL precision requires scaling to be maintained after additional emissions

# Logarithmic accuracy – Analytic proof

- Lorentz transformation defined by shift  $\tilde{K} \rightarrow K$

$$K^\mu = \tilde{K}^\mu - X^\mu, \quad \text{where} \quad X^\mu = p_j^\mu - (1-z)\tilde{p}_i^\mu$$

- $X$  is small, but is it small enough? Rewrite

$$\Lambda_\nu^\mu(K, \tilde{K}) = g_\nu^\mu + \tilde{K}^\mu A_\nu + X^\mu B_\nu$$

- In NLL limit, coefficients scale as

$$A^\nu \xrightarrow{\rho \rightarrow 0} 2 \frac{\tilde{K} X}{\tilde{K}^2} \frac{\tilde{K}^\nu}{\tilde{K}^2} - \frac{X^\nu}{\tilde{K}^2}, \quad \text{and} \quad B^\nu \xrightarrow{\rho \rightarrow 0} \frac{\tilde{K}^\nu}{\tilde{K}^2}.$$

- Simplify situation by taking  $a = 1, b = 0$  (worst offenders)

Relative momentum shift of soft emission particle  $l$  becomes

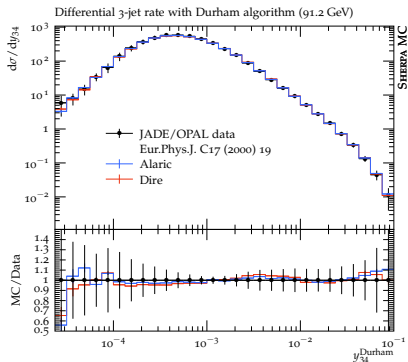
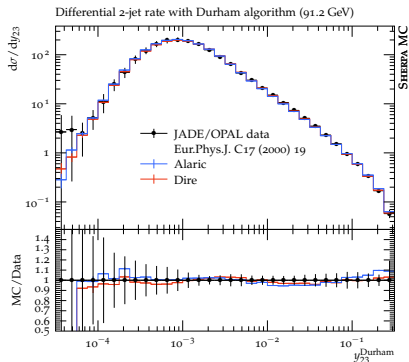
$$\Delta p_l^{0,3} / \tilde{p}_l^{0,3} \sim \rho^{1-\max(\xi_i, \xi_j)} \xrightarrow{\rho \rightarrow 0} 0$$

$$\Delta p_l^{1,2} / \tilde{p}_l^{1,2} \sim \rho^{1-\xi_i} \xrightarrow{\rho \rightarrow 0} 0$$

- For hard momenta, leading terms in  $X^\mu$  cancel exactly  
Remaining components scale as  $\rho$  or stronger

$$e^+e^- \rightarrow \text{hadrons}$$

[Herren,Krauss,Reichelt,Schönherr,SH] arXiv:2208.06057

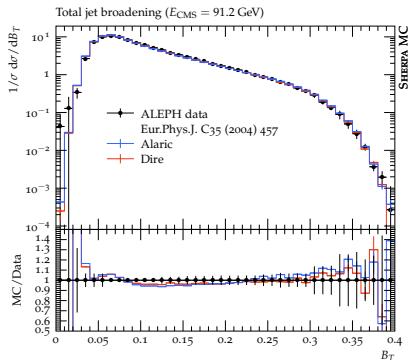
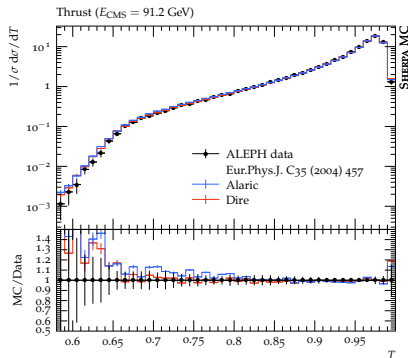


■ Comparison to experimental data from LEP



$$e^+e^- \rightarrow \text{hadrons}$$

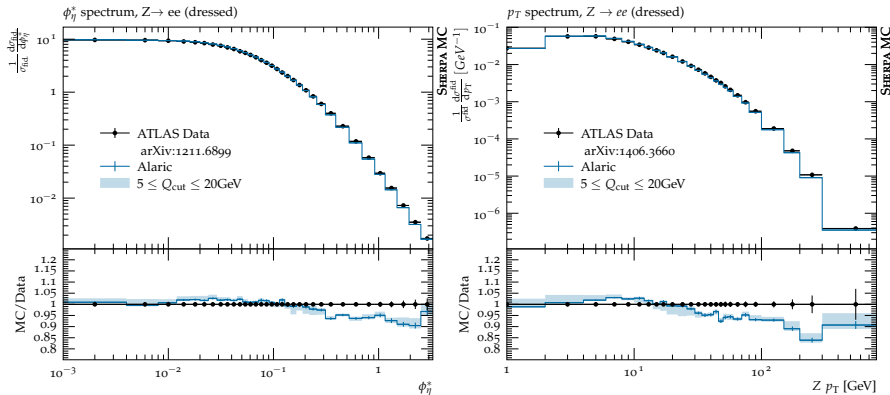
[Herren,Krauss,Reichelt,Schönherr,SH] arXiv:2208.06057



■ Comparison to experimental data from LEP

# Drell-Yan lepton pair production

[Krauss,Reichelt,SH] TBP



- Comparison to experimental data from LHC
- Leading-order multi-jet merging with up to two jets

# Heavy quark effects in parton showers

## A fresh perspective

# Experimental observations

- Example  $t\bar{t}b\bar{b}$ : MC single largest source of uncertainty on signal strength
- Despite intense study of HF production

- Fixed order, NLL, FONLL

[Cacciari,Frixione,Houdeau,Mangano,Nason,Ridolfi,...]  
 arXiv:1205.6344, hep-ph/0312132, hep-ph/9801375,  
 NPB373(1992)295

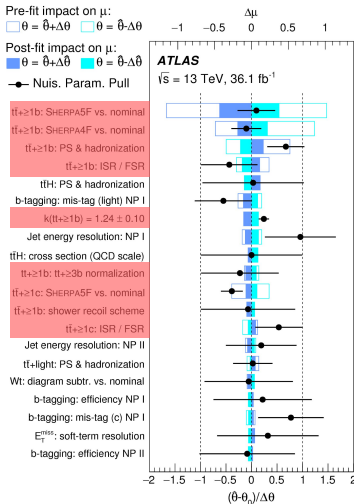
- In context of particle-level Monte Carlo

[Marchesini,Webber] NPB330(1990)261,  
 [Norrbin,Sjöstrand] hep-ph/0010012,  
 [Gieseke,Stephens,Webber] hep-ph/0310083,  
 [Schumann,Krauss] arXiv:0709.1027,  
 [Gehrmann-deRidder,Ritzmann,Skands] arXiv:1108.6172,  
 [Assi,SH] arXiv:2307.00728

- Recurring themes, not special to  $t\bar{t}b\bar{b}$

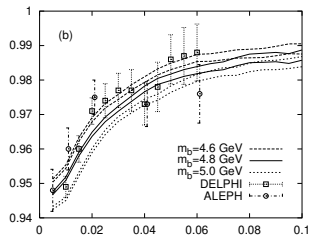
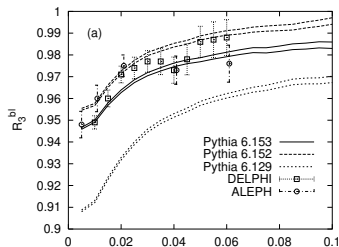
- PS uncertainties hard to judge and reduce  
 [Cascioli,Maierhöfer,Moretti,Pozzorini,Siegert] arXiv:1309.591
  - Matching needed for inclusive predictions  
 [Krause,Siegert,SH] arXiv:1904.09382,  
 [Ferencz,Katzy,Krause,Pollard,Siegert,SH]

[ATLAS] arXiv:1712.08895



# Theory problems

- Both high-energy limit and threshold region of heavy-flavor production to be modeled, but a number of obstacles:
- Infrared finite prediction for  $g \rightarrow Q\bar{Q}$  leaves splitting functions somewhat arbitrary
- Soft gluon emission off light/heavy quarks associated with  $\alpha_s(k_T^2)$ , i.e. “correct” scale is  $k_T^2$  [Amati et al.] NPB173(1980)429, but no such argument to set scale for  $g \rightarrow Q\bar{Q}$   
→ HQ production rate not very stable w.r.t. parton shower variations
- A number of different prescriptions, e.g.  
[Marchesini,Webber] NPB330(1990)261,  
[Norrbin,Sjöstrand] hep-ph/0010021,  
[Gieseke,Stephens,Webber] hep-ph/0310083,  
[Schumann,Krauss] arXiv:0709.1027,  
[Gehrmann-deRidder,Ritzmann,Skands] arXiv:1108.6172,  
[Assi,SH] arXiv:2307.00728



[Norrbin,Sjöstrand] hep-ph/0010021

# Soft-collinear matching for heavy quarks

[Marchesini,Webber] NPB330(1990)261

- Singularity in angular radiator screened by velocity  $\rightarrow$  deadcone  $\theta_0 \approx m/E$

$$W_{ik,j} = \frac{1 - v_i v_k \cos \theta_{ik}}{(1 - v_i \cos \theta_{ij})(1 - v_k \cos \theta_{jk})} - \frac{(1 - v_i^2)/2}{(1 - v_i \cos \theta_{ij})^2} - \frac{(1 - v_k^2)/2}{(1 - v_k \cos \theta_{jk})^2}$$

- Quasi-collinear divergence if  $m_Q \propto k_T$  as  $k_T \rightarrow 0$

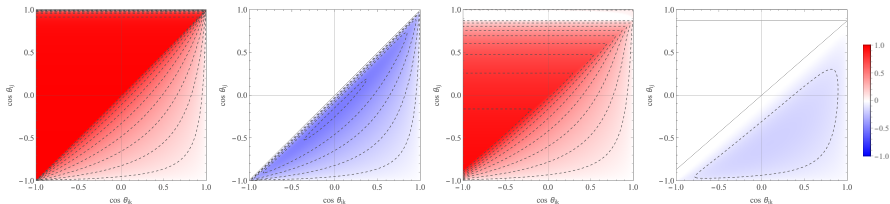
$\rightarrow$  Expose individual singularities via  $W_{ik,j} = \tilde{W}_{ik,j}^i + \tilde{W}_{ki,j}^k$

$$\tilde{W}_{ik,j}^i = \frac{1}{2(1 - v_i \cos \theta_{ij})} \left[ \left( \frac{1 - v_i v_k \cos \theta_{ik}}{1 - v_k \cos \theta_{kj}} - \frac{1 - v_i^2}{1 - v_i \cos \theta_{ij}} \right) + 1 - \frac{1 - v_i \cos \theta_{ij}}{1 - v_k \cos \theta_{kj}} \right]$$

- Approximate angular ordering after azimuthal averaging

$$v^2 = 1 - m_b^2/m_Z^2$$

$$v^2 = 1 - m_t^2/(350 \text{ GeV})^2$$



# A novel approach to heavy-quark evolution

[Assi,SH] arXiv:2307.00728

- Alternative approach: separate into energy & angle first

Partial fraction angular radiator only:  $W_{ik,j} = \bar{W}_{ik,j}^i + \bar{W}_{ki,j}^k$

$$\bar{W}_{ik,j}^i = \frac{1 - v_k \cos \theta_{kj}}{2 - v_i \cos \theta_{ij} - v_k \cos \theta_{kj}} W_{ik,j}$$

- Can be written in more intuitive form ( $n^\mu$  defines reference frame)

$$\bar{W}_{ik,j}^i = \frac{1}{2l_i l_j} \left( \frac{l_{ik}^2}{l_{ik} l_j} - \frac{l_i^2}{l_i l_j} - \frac{l_k^2}{l_k l_j} \right), \quad \text{where} \quad l_i^\mu = \sqrt{n^2} \frac{p_i^\mu}{p_i n}$$

- Quasi-collinear limit manifest

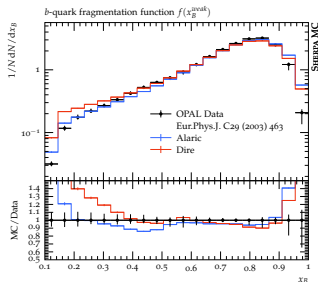
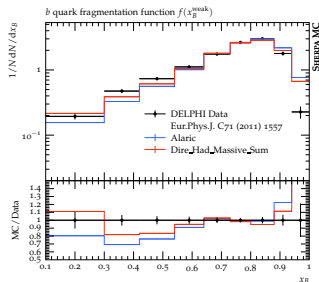
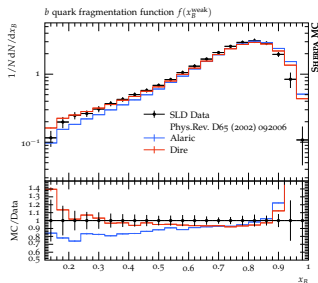
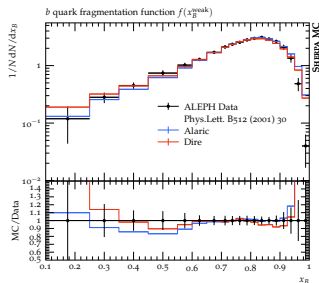
$$\frac{\bar{W}_{ik,j}^i}{E_j^2} \xrightarrow{m_i \ll p_i} w_{ik,j}^{(\text{coll})}(z) := \frac{1}{2p_i p_j} \left( \frac{2z}{1-z} - \frac{m_i^2}{p_i p_j} \right)$$

- Matching to massive DGLAP splitting functions

$$\frac{P_{(ij)i}(z, \varepsilon)}{(p_i + p_j)^2 - m_{ij}^2} \rightarrow \frac{P_{(ij)i}(z, \varepsilon)}{(p_i + p_j)^2 - m_{ij}^2} + \delta_{(ij)i} \mathbf{T}_i^2 \left[ \frac{\bar{W}_{ik,j}^i}{E_j^2} - w_{ik,j}^{(\text{coll})}(z) \right],$$

# A novel approach to heavy-quark evolution

[Assi,SH] arXiv:2307.00728





# A novel approach to heavy quark production

- Two different approaches to dealing with heavy-quark masses:
  - 4-flavor scheme (4FS): Decoupling scheme - (no  $b$ -quarks in PDF)
  - 5-flavor scheme (5FS): Minimal subtraction scheme
- Calculations can be matched by
  - Re-expressing both in same renormalization scheme
  - Subtracting the overlap

$$\sigma^{\text{FONLL}} = \sigma^{\text{massive}} + (\sigma^{\text{massless}} - \sigma^{\text{massive}, 0})$$

- This has been applied extensively to inclusive observables and is known as fixed-order next-to-leading log (FONLL) scheme

[Cacciari,Frixione,Mangano,Nason,Ridolfi] hep-ph/0312132,

[Forte,Napoletano,Ubiali] arXiv:1508.01529, arXiv:1607.00389, . . .

- Extension to differential observables is needed for MC simulations

# A novel approach to heavy quark production

[Krause,Siegert,SH] arXiv:1904.09382

## ■ Interpret $X + b\bar{b}$ as part of $X + jj$

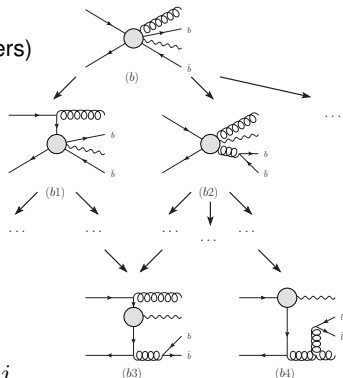
- 1 Cluster to obtain parton shower history
- 2 Apply  $\alpha_s(\mu_R^2) \rightarrow \alpha_s(p_T^2)$  reweighting
- 3 Apply Sudakov factors  $\Delta(t, t')$  (trial showers)

## ■ Remove double-counting

- 1 Cluster PS-level event using inverse PS
- 2 Look at leading two emissions
  - Heavy Flavour  $\rightarrow$  keep from  $Xb\bar{b}$  (“direct component”)
  - Light Flavour  $\rightarrow$  keep from  $X$ +jets (“fragmentation component”)
  - Subleading  $g \rightarrow b\bar{b}$  splittings not from  $Xb\bar{b}$  ME, but  $X4j$  ME+PS

## ■ Match 5F $\rightarrow$ 4F in PDFs and $\alpha_s$

- 1 Use 5F PDF /  $\alpha_s$  to be consistent with  $Xjj$
- 2 Use matching coefficients to correct to 4F scheme  
[Buza,Matiounine,Smith,van Neerven] hep-ph/9612398, [Forte,Napoletano,Ubiali] arXiv:1607.00389  
 $\rightarrow$  Coefficients up to (N)LL generated by (N)LO parton shower!
- 3 Reweighting needed only for  $\alpha_s$  in hard ME

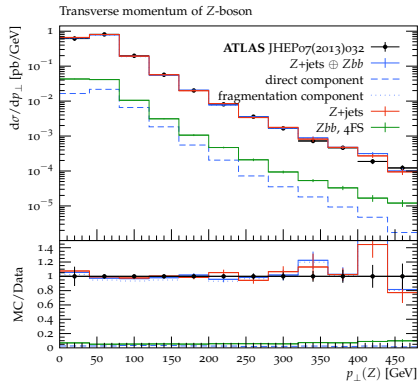


Can be applied to LO and NLO merging!

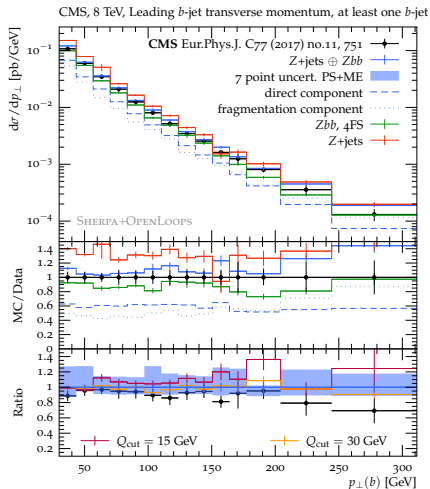
# Application to $Z$ +jets & $Zb\bar{b}$

## Validation with LHC data

[Krause,Siegert,SH] arXiv:1904.09382



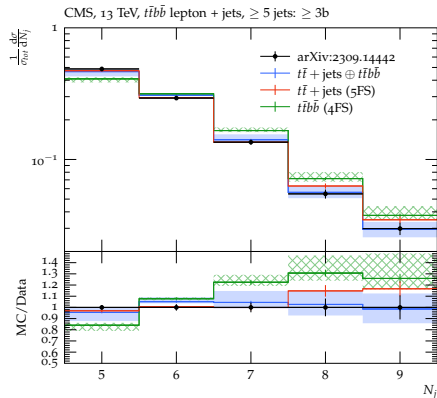
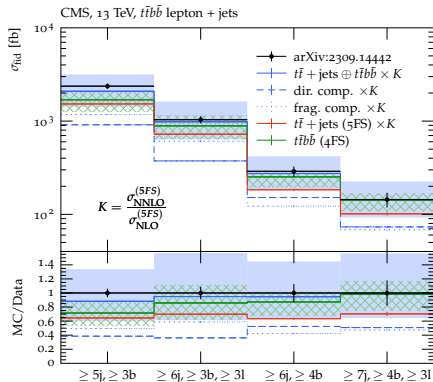
	Data [pb]	Fusing [pb]
$Z+ \geq 1b$	$3.55 \pm 0.24_{\text{comb}}$	$3.80(5) \pm 0.33$
$Z+ \geq 2b$	$0.331 \pm 0.037_{\text{comb}}$	$0.282(4) \pm 0.022$



# Application to $t\bar{t}+jets$ & $t\bar{t}b\bar{b}$

[J. Krause] PhD thesis, [Ferencz,Katzy,Siegert,SH] arXiv:2402.15497

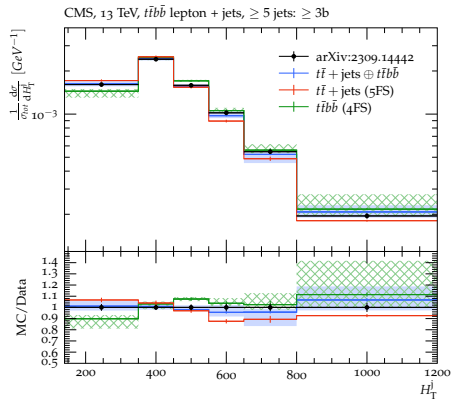
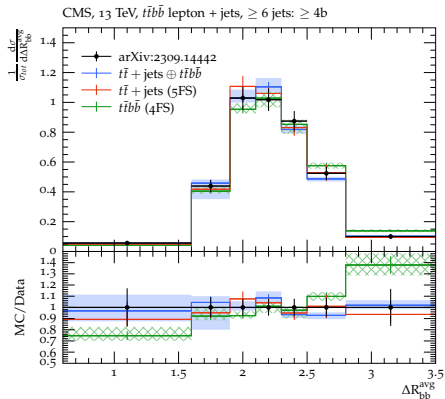
- Combination of  $t\bar{t}+0,1j@NLO+2,3j@LO$  and massive  $t\bar{t}b\bar{b}@NLO$
- 2-bjet production dominated by precise calculation of direct component



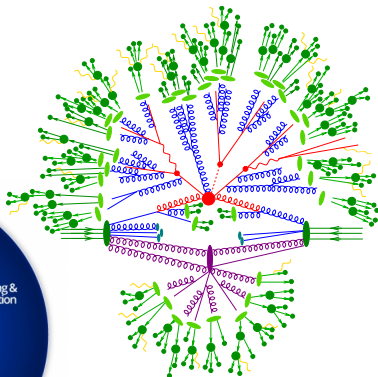
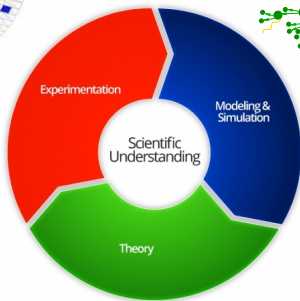
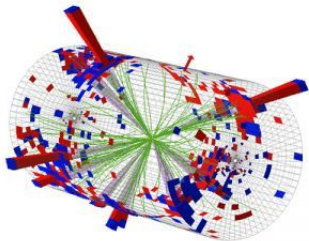
# Application to $t\bar{t} + \text{jets}$ & $t\bar{t}b\bar{b}$

[J. Krause] PhD thesis, [Ferencz,Katzy,Siegert,SH] arXiv:2402.15497

- Combination of  $t\bar{t} + 0, 1j @ \text{NLO} + 2, 3j @ \text{LO}$  and massive  $t\bar{t}b\bar{b} @ \text{NLO}$
- 2-bjet production dominated by precise calculation of direct component



# Half a century of teamwork ...



$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\Psi}\not{D}\Psi + h.c.$$

## ... and we're only getting started

- Fixed-order calculations (not covered here)
  - Higher-order matrix element calculations
  - Higher-order fully differential IR subtraction
  - Computing improvements
- Parton showers
  - Improved logarithmic precision
  - Higher-order splitting kernels
  - Interplay with analytic resummation
- Matching and merging
  - The role of unitarity constraints
  - Interplay with analytic resummation
  - Fully differential higher-order matching

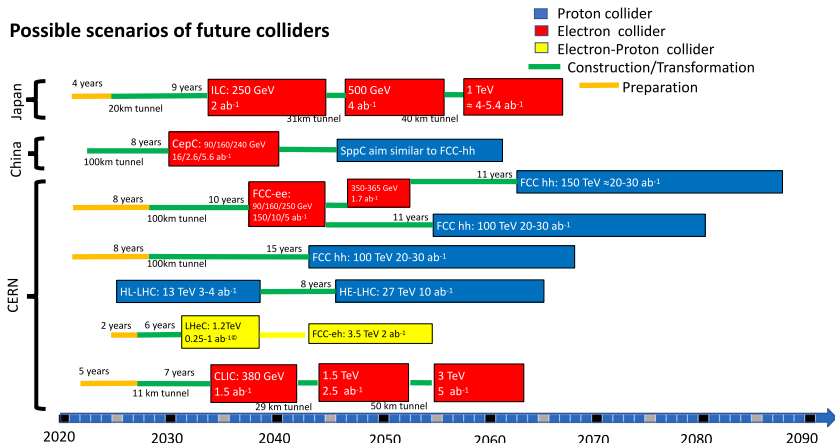
Apologies for only selecting a small subset of topics

For a comprehensive overview: [\[Campbell et al.\] arXiv:2203.11110](#)

# Whatever the future may hold ...

[Gray] Rev.Phys. 6 (2021) 100053

## Possible scenarios of future colliders





## ... nothing goes without simulations

