

# **QCD Theory meets Information Theory**

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### Outline

Improving Monte-Carlo simulations:

- 1) Motivation and brief review of parton showers
- 2) Higher precision QCD Theory control
- 3) Information Theoretic event-level re-weighting
- 4) Machine learning for hadronization (very briefly)





# **Quantifying precision**

Current status of (resummed) perturbative precision in QCD

Drell-Ya	n (γ/Z)	& Higg	s productio	on at ha	adron coll	iders		
LO		NLO	NLO		[	]	N3LO	
	DGLA	AP split	ting function	ons (us	ed in PDF	-s)		
	LO	NLO				NNLO	[parts c	of N3LO
		transverse-momentum resummation (DY&Higgs)						
			NLL[]			NNLL[]	N3LL	
			parton sho	owers	(many of t	oday's widely-used sho	owers only LL@leading	-colour)
			LL	[parts	of NLL		]	
					fixed-ord	er matching of p	rton showers	
					LO	NLO	NNLO []	[N3LO]
1970	1	1980	19	90	20	00 20	10 20	)20

G. Salam, Moriond 2023

# **Quantifying precision**

Current status of (resummed) perturbative precision in QCD



### **Generators are among us**



Keith Hamilton (2021)

# **Factorizing QCD**



### Anatomy of a high-energy collision



#### **Parton Shower**

**Mechanism:** Gluon emission  $\leftrightarrow$  dipole splitting at large  $N_c$ 

Branching requires going from a more massive to a less massive state

Energy is taken to boost the mass but should not affect the event topology (angles & relative separation)

Parton masses must **stay the same** before and after branching

Careful **momentum mapping** needed from pre- to post-branching



### **Beyond Leading Accuracy**

NLL **accurate** if emissions factorise up to  $\mathcal{O}(e^{-\Delta})$  corrections

Emissions should be **wellseparated** in the Lund plane

How to test whether true NLL deviations or subleading effects?

#### Resummation regime

 $\alpha_s \log v \sim 1, \ \alpha_s \ll 1$ 

Banfi, Salam, Zanderighi JHEP 03 (2005)



# An NLL accurate algorithm in SHERPA

**ALARIC** momentum mapping:

**Recoil** compensated **globally** by neg. sum of multipole momenta  $\tilde{K}$  including splitter

K receives kick of  $\mathcal{O}(k_{\perp})$  from the emission that can be understood as a Lorentz TF

Since *K* chosen such that  $K^2 \gg k_{\perp}^2$  it does **not** affect topology of **previous emissions** in the Lund plane because its effect scales as  $k_{\perp}^2/K^2$ 

**Uniquely** analytically provable that this algorithm is **NLL accurate** 

Herren, Höche et al. JHEP 10 (2023) BA, Höche PRD 109 (2024)





#### $B_T$

### Subtleties of heavy flavour evolution

Both **high-energy** and **threshold** regime require accurate descriptions

Multiple prescriptions - varying success in describing experiments

Norrbin, Sjöstrand; Gieseke, Stephens; Schumann, Krauss; Gehrmann-deRidder, Ritzmann, Skands

Required for proper description of bottom and charm jet production and quark **fragmentation functions** 

**Generalising ALARIC** for massive flavours: careful analysis of the branching probabilities, matching of soft & quasi-collinear limits, NLO matching (complicated integrals)

BA, Höche PRD 109 (2024)



Norrbin, Sjöstrand hep-ph/0010012

### **Experimental comparison**



**Better agreement** for Alaric predictions with experimental data (same had. tune)

#### **Towards Higher Orders**

Calculated NLO matching in both massive and massless case  $\Rightarrow$  next step is **implementation** BA, Höche, *In preparation* 

Towards MC @ NNLO fully integrated generator - need NNLO subtraction scheme - NSCS scheme matches ALARIC construction BA, Höche, Campbell, Röntsch,...

Many **more improvements** to ALARIC: spin correlations, full color treatment, higher multiplicities, complete NNLL, etc.

# Can we incorporate higher precision theory information?



#### **QCD Theory meets Information Theory**

Boltzman machine: Generative model samples according to stat dist

$$P(\mathbf{s}) \sim e^{-E/T}, \quad E = -\sum_{i < j} w_{ij} s_i s_j - \sum_i \theta_i s_i$$

Boltzman factor: Maximum entropy solution subject to constraint on average energy

$$p(x) = q(x) \exp \begin{bmatrix} -\beta_0 - \beta_1 f_1(x) - \beta_2 f_2(x) - \dots \end{bmatrix} \xrightarrow{\text{HEP}} \underbrace{\text{HEP}}_{\text{Lagrange Multipler}} \underbrace{\text{Constrained Quantity}}_{\text{Constrained Quantity}}$$

Sudakov structure: Plucking a random event-shape observable distribution

$$r(\tau)_{\rm LL, f.c.} = \frac{-2\alpha_s C_F}{\pi} \frac{\ln \tau}{\tau} \exp\left[-\frac{\alpha_s C_F}{\pi} \ln^2 \tau\right]$$
  
Sudakov factor

**ML practitioner:** Sudakov = Boltzmann factor and cusp AD = Lagrange multiplier that enforces constraint on the 2nd log moment of distribution

log moments not previously measured or calculated before in QCD!



#### **QCD** Theory meets Information Theory

Start with **relative entropy** 

Take analytic **constraints** from precision QCD theory

$$\mathcal{L}_{\mathrm{KL}}(p \parallel q) = \int d\Phi \, p(\Phi) \ln \frac{p(\Phi)}{q(\Phi)}$$

$$c_j[r] = \int dec v \, r(ec v) \, g_j(ec v) \,, \quad d_j[p] = \int d\Phi \, p(\Phi) \, g_jig(ec v(\Phi)ig)$$

Relative entropy under constraints

$$\mathcal{L}[p,q] = \mathcal{L}_{\mathrm{KL}}(p \parallel q) + \sum_{j} \lambda_j (c_j[r] - d_j[p])$$

Minimised if prior (generator) distribution is modified as

 $p(\Phi) = q(\Phi) w(\Phi) , \quad w(\Phi) \equiv \exp\left[-\sum_{j} \lambda_{j} g_{j}(\vec{v}(\Phi))\right]$ 

**Note:** Weights strictly positive!



BA, Höche, Lee, Thaler 2501.17219

# An example of thrust



BA, Höche, Lee, Thaler 2501.17219

Choice of moment basis relevant to improve **different physical regions** (perturbative, Sudakov peak, Sudakov shoulder,...) and largely **independent** of MC priors

# Impact on other observables



0.15

Α

# **QCD Theory meets Information Theory**

#### **Proof-of-Concept with Diverse Priors:**

Validated with 4 *priors* combining 2 showers (CSShower, Dire) and 2 hadronization models (Pythia8, Ahadic)

#### **Improved Accuracy & Convergence:**

Scale uncertainty bands and convergence from LL to NNLL + NNLO accuracy!

#### **Natural Uncertainty Propagation:**

Propagate moment uncertainties directly to Lagrange multipliers

**Further improvement** systematically attainable by including additional moments and **precision observables** 

BA, Höche, Lee, Thaler 2501.17219



### Can we achieve yet higher precision?

Incorporate **combined** theory information:  $N^3LO W/Z p_T$  from MCFM and high precision angular observables

BA, Campbell, Höche, Lee, Thaler, In preparation

Higher order available resummed observables e.g. EECs at N<sup>4</sup>LL & ab-initio Lattice QCD input

Avkahdiev, Shanahan, Wagman, Zhao: hep-lat/2402.06725

**Big goal:** Precise  $\alpha_s$  extraction with maximal accounting of theory uncertainties!

# What about Non-Perturbative Dynamics?

# **Machine Learning for Hadronization**

#### **MLHad collaboration**

(Pythia-based) since joining UC of 9 theorists and experimentalists

**Big goal**: Develop a datadriven, ML-based framework with max theory information for simulating hadronization in event generators (compare NNPDF)





BA, Bierlich, Ilten, Menzo, Mrenna, Szwec, Wilkinson, Youssef, Zupan



### **Factorizing QCD**



#### Shape of an emission

#### **Emission:**

$$(\tilde{p}_q, \tilde{p}_{\bar{q}}) \to (p_q k, k p_{\bar{q}})$$

with  $k^{\mu} = z_q \tilde{p}^{\mu}_q + z_{\bar{q}} \tilde{p}^{\mu}_{\bar{q}} + k^{\mu}_t$ 

#### **Degrees of freedom:**

1) Rapidity: 
$$\eta = \frac{1}{2} \log \frac{z_q}{z_{\bar{q}}}$$
  
2) Transverse momentum:  $k_t$   
3) Azimuth:  $\phi$ 



# **Beyond Leading Accuracy**

#### **Evolution steps:**

- 1) Generate  $k_{t,1} < Q$  with Sudakov probability
- 2) Generate  $\eta_1$  and split dipoles  $(q\bar{q}) \rightarrow (qg_1) + (g_1\bar{q})$
- 3) Generate  $k_{t,2} < k_{t,1}$  from 2 dipoles
- 4) Generate  $\eta_2$  and split dipoles  $(g_1\bar{q}) \to (\bar{q}g_1) + (g_1g_2)$
- 5) Iterate until  $k_t = k_{t,\text{cut}}$



 $\uparrow \log k_t$ 

Banfi, Salam, '17

### An NLL accurate algorithm in SHERPA



Herren, Höche, Krauss, BA, Höche,

### **Massive NLL accurate algorithm in SHERPA**

Ingredient 1: Treatment of soft radiation

Matrix element factorizes in soft gluon limit

$$|M|^{2} \propto \frac{2W_{ik,j}}{E_{j}^{2}} = \frac{2}{E_{j}^{2}} \frac{(1 - \cos \theta_{ik})}{(1 - \cos \theta_{ij})(1 - \cos \theta_{jk})} - \frac{p_{i}^{2}}{(p_{i}p_{j})^{2}} - \frac{p_{k}^{2}}{(p_{k}p_{j})^{2}}$$

Avoid soft double-counting by partial fractioning

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

**Ingredient 2:** Momentum mapping maintain directions and collinear safety upon emission

Recoil compensated **globally** by sum of multipole momenta  $\tilde{K}$ 

$$\begin{split} p_i^{\mu} &= \ \bar{z} \ \frac{\tilde{p}_{ij}^{\mu} - \bar{\mu}_{ij}^2 \tilde{K}^{\mu}}{\bar{z}_{ij} v_{\tilde{p}_{ij},\tilde{K}}} + \left( y(1 - \bar{z})(1 + \mu_{ij}^2 - \mu_i^2 - \mu_j^2) - \bar{z}(\mu_i^2 + \mu_j^2) + 2\mu_i^2 \right) \frac{\tilde{K}^{\mu} - \bar{\kappa} \, \tilde{p}_{ij}^{\mu}}{v_{\tilde{p}_{ij},\tilde{K}} / z_{ij}} + k_{\perp}^{\mu} \\ p_j^{\mu} &= \ (1 - \bar{z}) \ \frac{\tilde{p}_{ij}^{\mu} - \bar{\mu}_{ij}^2 \tilde{K}^{\mu}}{\bar{z}_{ij} v_{\tilde{p}_{ij},\tilde{K}}} + \left( y \, \bar{z} \, (1 + \mu_{ij}^2 - \mu_i^2 - \mu_j^2) - (1 - \bar{z})(\mu_i^2 + \mu_j^2) + 2\mu_j^2 \right) \frac{\tilde{K}^{\mu} - \bar{\kappa} \, \tilde{p}_{ij}^{\mu}}{v_{\tilde{p}_{ij},\tilde{K}} / z_{ij}} - \frac{1}{2} \end{split}$$

Previous emissions are only mildly affected by the boost which is the basis of the **analytic proof** of NLL accuracy







#### BA, Höche,

#### Subtraction at NLO — Soft integrals

E.g. Integral with two massive denominators given by

$$\begin{split} I_{1,1}^{(2)}(v_{11}, v_{12}, v_{22}) &= \frac{\pi}{\sqrt{v_{12}^2 - v_{11}v_{22}}} \left\{ \log \frac{v_{12} + \sqrt{v_{12}^2 - v_{11}v_{22}}}{v_{12} - \sqrt{v_{12}^2 - v_{11}v_{22}}} + \epsilon \left( \frac{1}{2} \log^2 \frac{v_{11}}{v_{13}^2} - \frac{1}{2} \log^2 \frac{v_{22}}{v_{23}^2} \right) \right. \\ &+ 2 \text{Li}_2 \left( 1 - \frac{v_{13}}{1 - \sqrt{1 - v_{11}}} \right) + 2 \text{Li}_2 \left( 1 - \frac{v_{13}}{1 + \sqrt{1 - v_{11}}} \right) \\ &- 2 \text{Li}_2 \left( 1 - \frac{v_{23}}{1 - \sqrt{1 - v_{22}}} \right) - 2 \text{Li}_2 \left( 1 - \frac{v_{23}}{1 + \sqrt{1 - v_{22}}} \right) \right) + \mathcal{O}(\epsilon^2) \bigg\} \end{split}$$

Massless limit only one simpler integral [arXiv:2208.06057]

$$I_{1,1}^{(1)}(v_{12}, v_{12}) = -\frac{\pi}{v_{12}^{1+\epsilon}} \left\{ \frac{1}{\epsilon} + \epsilon \operatorname{Li}_2\left(1 - v_{12}\right) + \mathcal{O}(\epsilon^2) \right\}$$

# SIMPLIFIED STRING HADRONIZATION MODEL

- assume that color flow done correctly by Pythia
  - including splitting gluons, so that only strings with  $q, \bar{q}$  ends
- hadron emission from a string piece controlled by fragmentation function f(z)
  - the whole hadronization chain is then reproduced by iterating
  - the string is labeled by  $q, \bar{q}$  flavor and its energy in cms, 2E
- for now only *u*,*d* quarks, uses Pythia flavor selector

