QCD simulations and Monte Carlo

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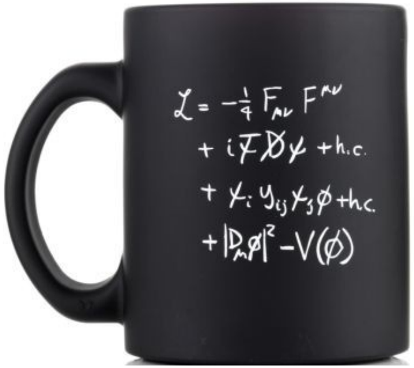
Disclaimer

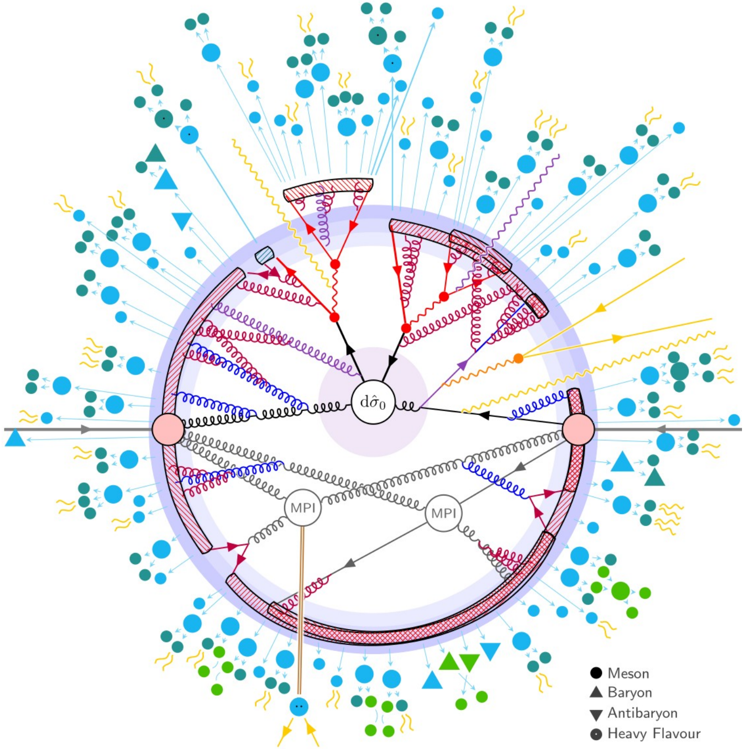
This talk summarizes mostly work I haven't been participating in personally
→ apologies in advance for any misrepresentation, omissions, mistakes, and personal biases…

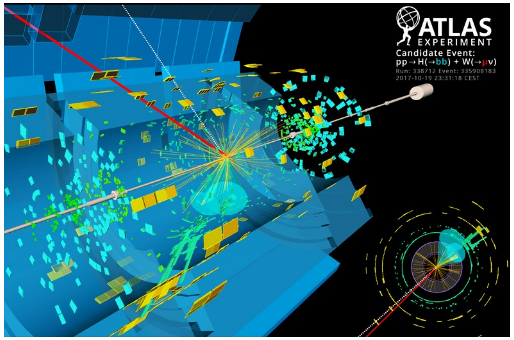
This is an overview with technicalities kept at a minimum,
but we have many experts here giving talks in the working groups!

Monte Carlo Event Generators

… the **bridge** between "theory world" and "real world"







[Pythia 8.3]

Scale factorization in collision events

Guiding physics principle
"What you see depends on the resolution"

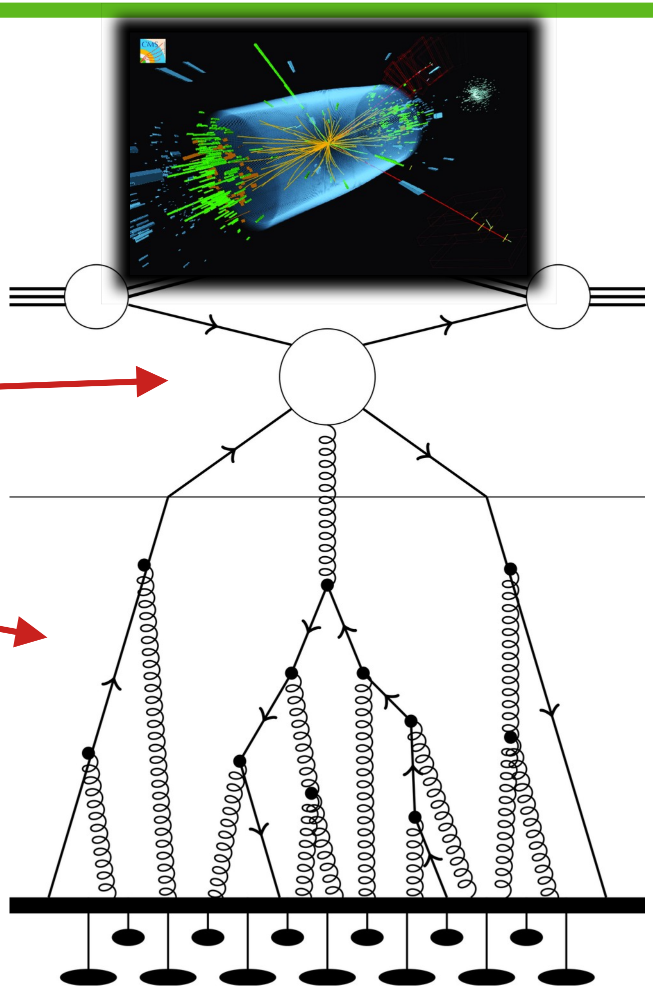
Example: Quantum Chromodynamics (QCD)

$Q \gg \Lambda_{\mathrm{QCD}}$ **Fixed-order perturbation theory**

$Q \gtrsim \Lambda_{\mathrm{QCD}}$ **Parton-shower/Resummation**

$Q \sim \Lambda_{\mathrm{QCD}}$ **"Hadronization"/MPI/…**

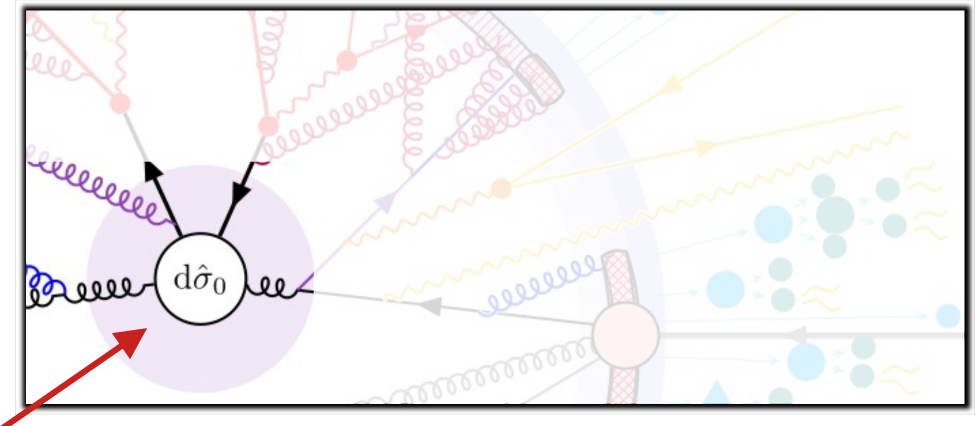
Energy



The tasks of Monte Carlo Event Generators

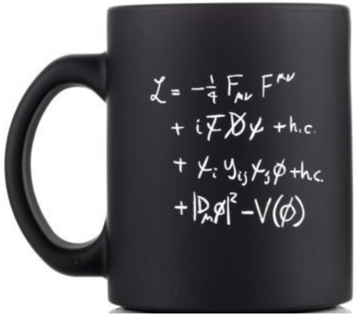
Energy

$Q \gg \Lambda_{\mathrm{QCD}}$

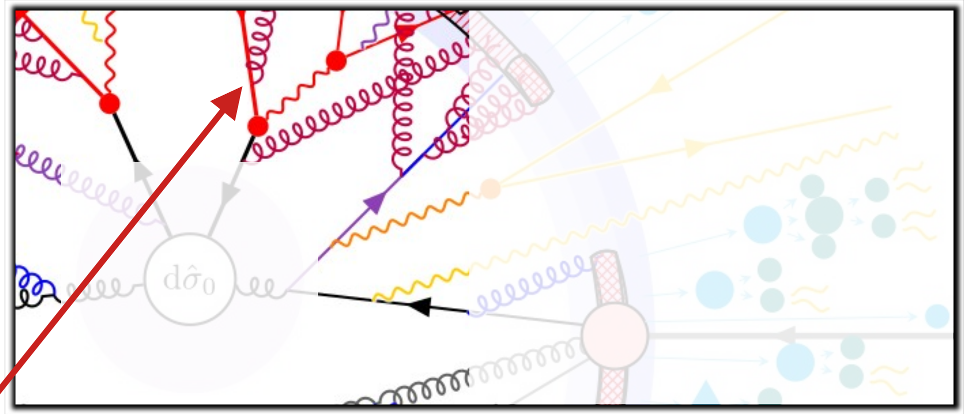


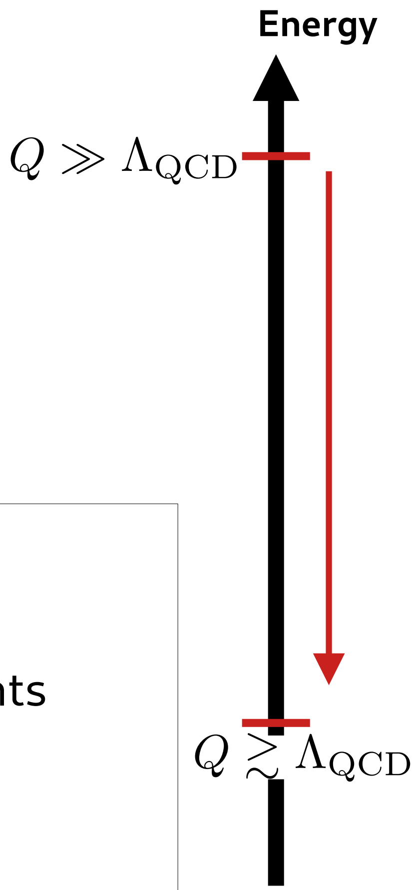
Hard scattering process

- Individual partons scatter at high momentum transfer
- Matrix elements directly from Lagrangian
- Fixed-order perturbation theory controls precision
  → expansions in orders of QCD and EW couplings



The tasks of Monte Carlo Event Generators

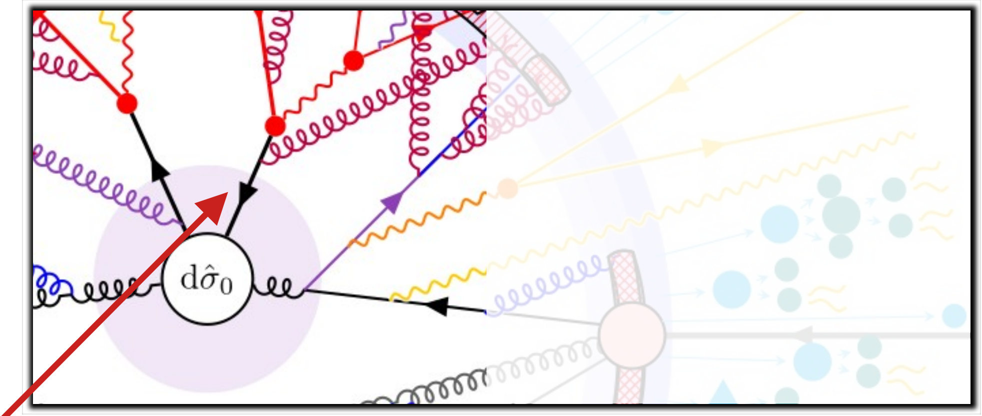


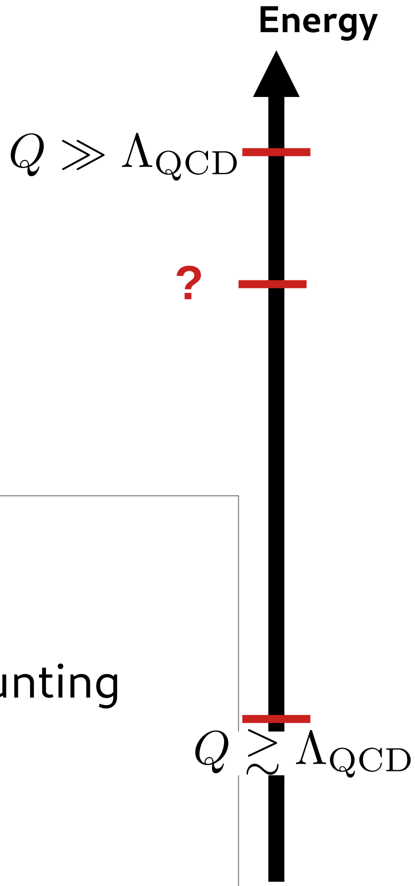


Parton-shower evolution

- Multi-particle radiation interpreted as a sequence of parton splittings
- Splitting probabilities → soft/collinear approximations of matrix elements
- all-order resummation, accuracy measured in resummed logarithms
- Accuracy controlled by:
  splitting functions, kinematics, treatment of color & spin

The tasks of Monte Carlo Event Generators

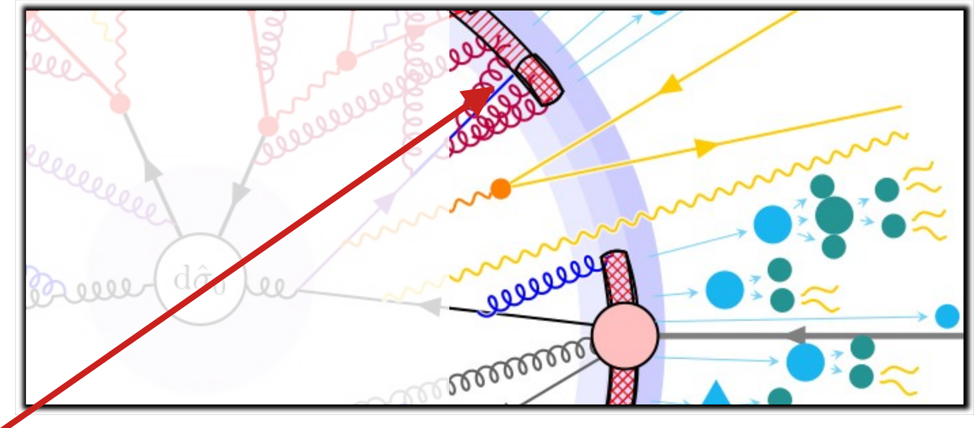


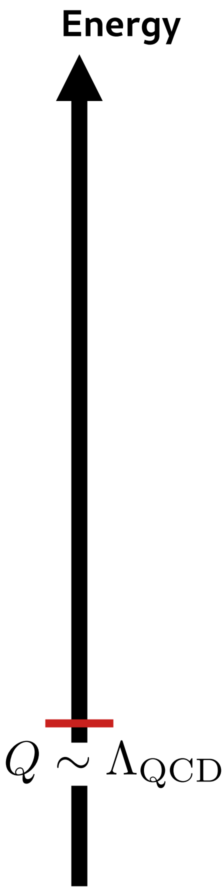


Matching/Merging

- combine hard scattering and parton-shower
- tricky bit: how to preserve the **precision/accuracy** and avoid double counting
- solve pathologies of higher fixed-order computations

The tasks of Monte Carlo Event Generators





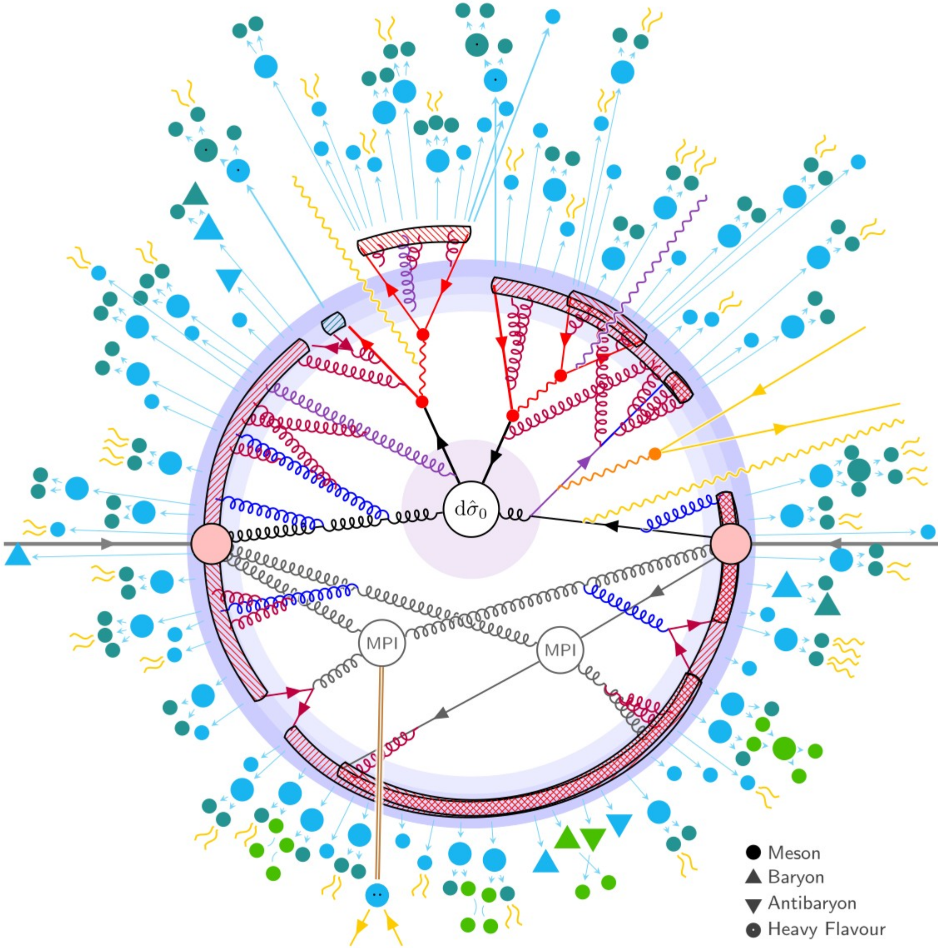
Hadronization

- Formation and decay of observable particles
- Intrinsically non perturbative physics
  → driven by phenomenological models
  → input from experiments

The tasks of Monte Carlo Event Generators

Global event considerations
- underlying event
- color reconnection
- multi parton interactions (MPI)
- beam remnants
- ...

Technical aspects
- Performance
- Tuning
- Uncertainties



LHC Era Monte Carlo Generators

[table shamelessly copied from S. Plätzer]

	Hard matrix elements	Shower algorithms	NLO Matching	Multi-jet merging	MPI	Hadronization	Shower variations
Herwig 7 [Eur.Phys.J.C 84 (2024)]	Internal, libraries, event-files	Qtilde, Dipoles	Internally automated	Internally automated	Eikonal	Cluster, (Strings)	Yes
Pythia 8 [SciPost Phys.Codeb. (2022)]	Internal, event-files	PT ordered, VINCIA	External	Internal, ME via event files	Interleaved	Strings	Yes
Sherpa 3 [JHEP 12(2024)]	Internal, libraries	CSShower, Alaric (future)	Internally automated	Internally automated	Eikonal	Clusters, Strings	Yes

The physics to describe is complicated: **methodological diversity is key** to **understand systematics** and to **validate** → relying on a single MC is asking for trouble…

Hot topics of MC development (a personal selection)

$Q \gg \Lambda_{\mathrm{QCD}}$

Fixed-order perturbation theory
→ automatise state-of-the-art (N)NNLO
→ matching to parton-shower (NNLO+PS)

$Q \gtrsim \Lambda_{\mathrm{QCD}}$

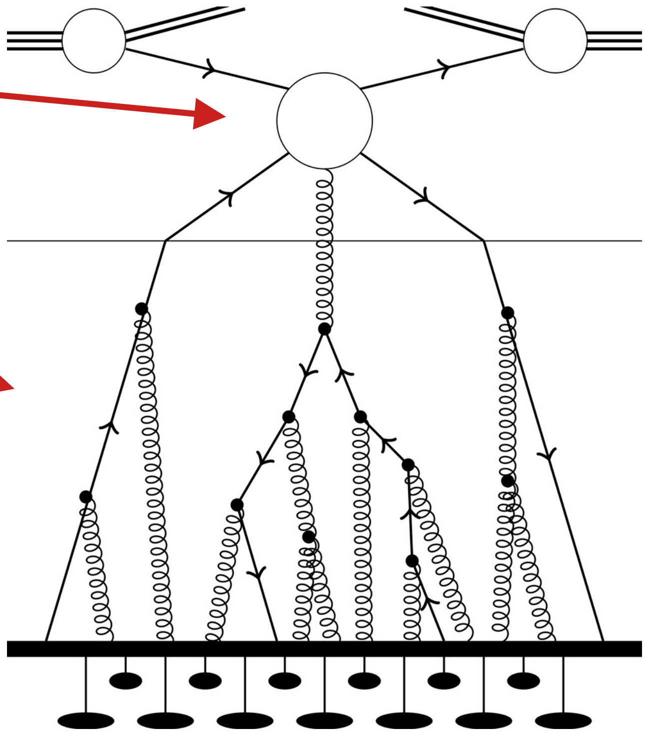
Parton-shower/Resummation
increasing parton-shower accuracy
→ NLL and towards (N)NLL
→ beyond leading color

$Q \sim \Lambda_{\mathrm{QCD}}$

"Hadronization"/MPI/...
→ refinement of models
→ improving constraints

General
→ efficiency improvement through ML

Energy

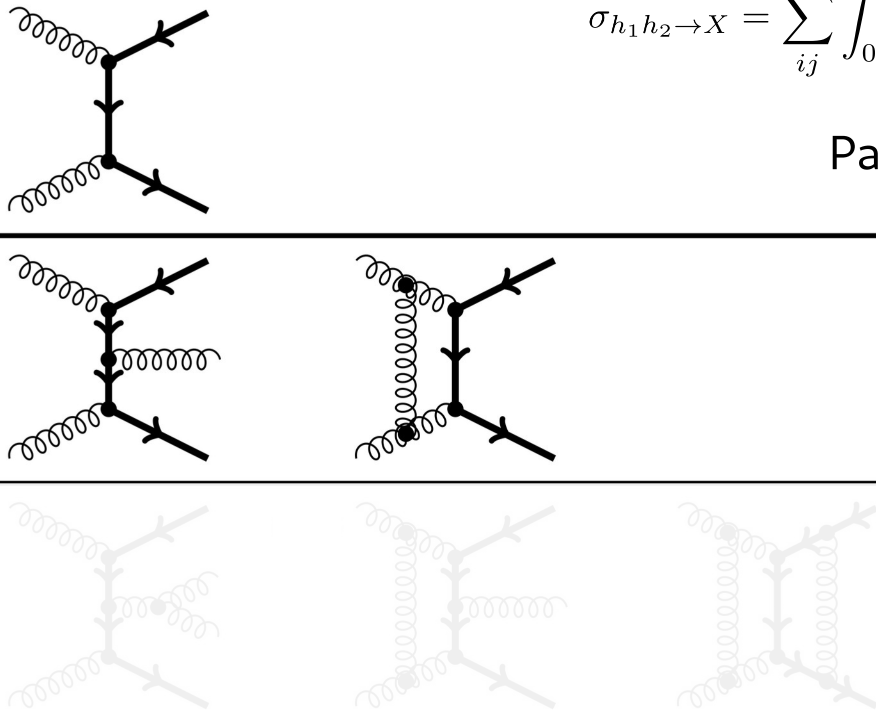


Fixed-order QCD in collinear factorization

LO

NLO

NNLO



$$\sigma_{h_1 h_2 \to X} = \sum_{ij} \int_0^1 \int_0^1 \mathrm{d}x_1 \mathrm{d}x_2 \phi_{i,h_1}(x_1, \mu_F^2) \phi_{j,h_2}(x_2, \mu_F^2) \hat{\sigma}_{ij \to X}(\alpha_s(\mu_R^2), \mu_R^2, \mu_F^2)$$

Parton distribution functions

→ see WG1 talks

Partonic cross section:

$$\hat{\sigma}_{ab\to X} = \hat{\sigma}^{(0)}_{ab\to X} + \hat{\sigma}^{(1)}_{ab\to X} + \hat{\sigma}^{(2)}_{ab\to X} + \mathcal{O}(\alpha_s^3)$$

Automated fixed-order computations @ NLO:

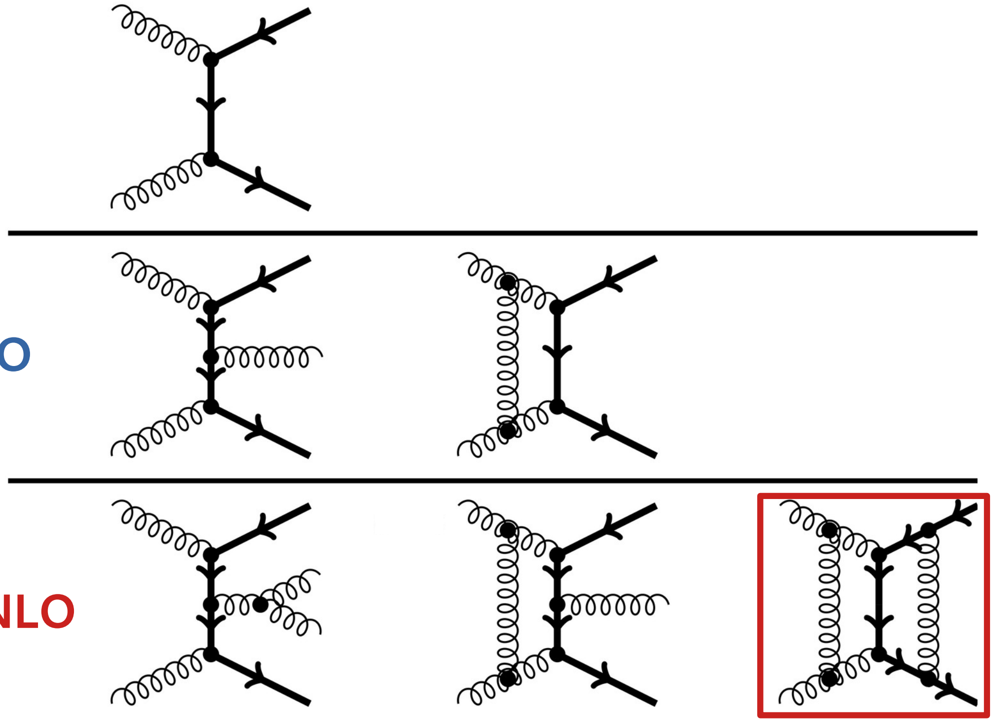
- Automated evaluation of loop-matrix elements:
  - Openloops, Recola, Helac, MadGraph, GoSam
- Modern automation of NLO QCD/EW subtraction:
  - FKS: MadGraph5_aMC@NLO, Powheg
  - CS dipoles: Sherpa, Herwig

NNLO QCD challenges: two-loop amplitudes

LO

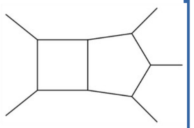
NLO

NNLO

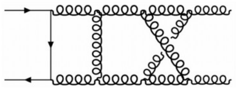


How to compute
multi-scale two-loop QCD amplitudes?
→ **fast growing complexity**:
rational coef. and **special functions**
→ deeper understanding of the analytical properties
→ refinement of computational tools

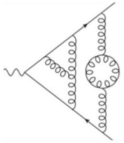
Two-loop 5-point
[Abreu, Agarwal, Badger, Buccioni, Chawdhry, Chicherin,Czakon, de Laurenties, Febres-Cordero, Gambuti, Gehrmann, Henn, Lo Presti, Manteuffel, Ma, Mitov, Page, Peraro, Poncelet, Schabiner Sotnikov, Tancredi, Zhang,...]



Three-loop 4-point
[Bargiela, Dobadilla, Canko, Caola, Jakubcik, Gambuti, Gehrmann, Henn, Lim, Mella, Mistleberger, Wasser, Manteuffel, Syrrakow, Smirnov, Trancredi, ...]



Four-loop 3-point
[Henn, Lee, Manteuffel, Schabinger, Smirnov, Steinhauser,...]



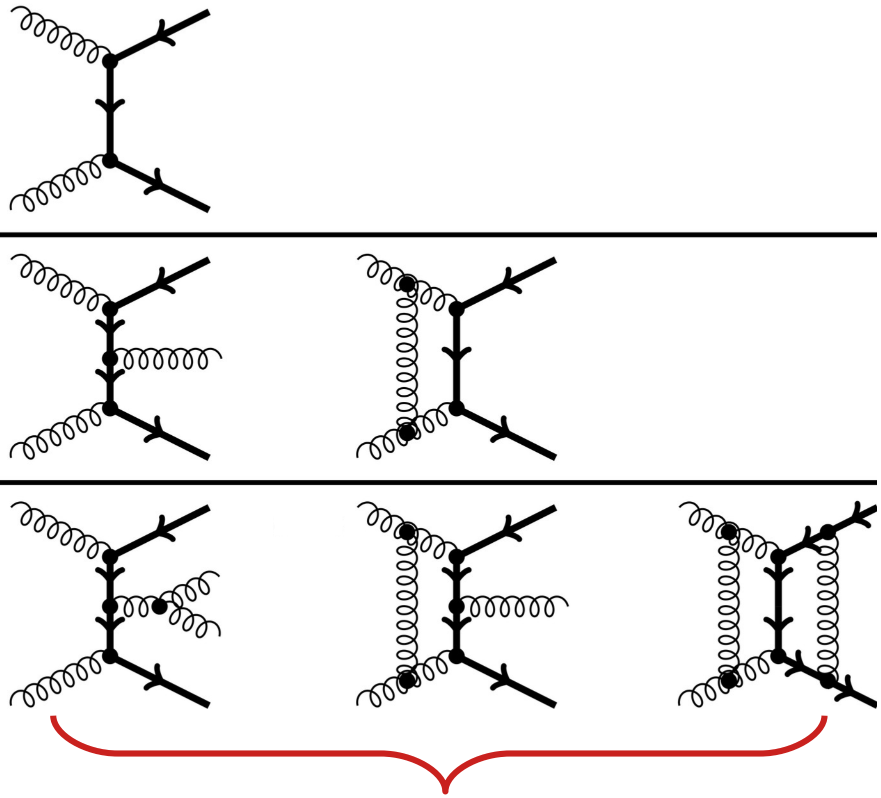
Great progress, however, one-loop-like automation still a open question

NNLO QCD challenges: subtraction

LO

NLO

NNLO



IR-finite cross section

How to achieve **infrared (IR) finite differential** cross sections at NNLO QCD?

~20 years to solve this problem

qT-slicing [Catani'07], N-jettiness slicing [Gaunt'15/Boughezal'15], Antenna [Gehrmann'05-'08], Colorful [DelDuca'05-'15], Projetction [Cacciari'15], Geometric [Herzog'18], Unsubtraction [Aguilera-Verdugo'19], Nested collinear [Caola'17], Local Analytic [Magnea'18] Sector-improved residue subtraction [Czakon'10-'14,'19]

NNLO QCD Automation

→ qT-slicing (massive/color singlet) in MATRIX & MCFM (public)
→ Antenna subtraction (NNLOJet → public)
→ Sector-improved residue subtraction (private impl.)
→ color singlets with nested-collinear: history

First fully differential N3LO

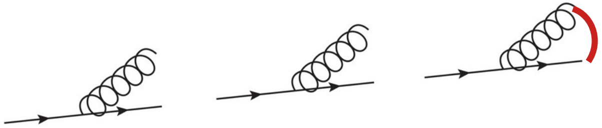
→ combination of qT-slicing + NNLO local subtraction for pp
→ antenna for final state only

→ Tiziano Peraro's talk

Beyond Leading Order: The Need for Matching

The challenge

Combine fixed-order with parton shower evolution
while **preserving** the precision/accuracy of both!

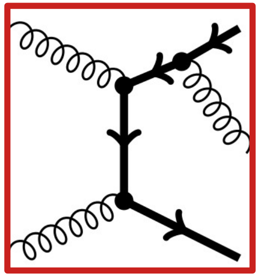


v ← shower scale

parton shower approximation: $\alpha_S^i(v)\ln^j(v)$
but to all orders!

accuracy: LL, NLL, NNLL, ...

“Hard” scattering scale Q



Fixed-order: expansion in $\alpha_S(Q)$

→ cross section ~ $\underbrace{e^{\sum_{ij}\alpha_S^i(v)\ln^j(v)} \times (\mathrm{LO} + \mathrm{NLO} + \mathrm{NNLO} + \dots)}$

A matching scheme needs to avoid double counting
of the logarithmic contributions!

Beyond Leading Order: The Need for Matching

NLO + Parton Shower Matching

- Standard tools: **POWHEG** and **MC@NLO**
- Implemented in all major frameworks: Herwig, SHERPA, Madgraph, Powheg-box,...
- Standard for most LHC analyses today.

Current state-of-the-art: NNLO+PS

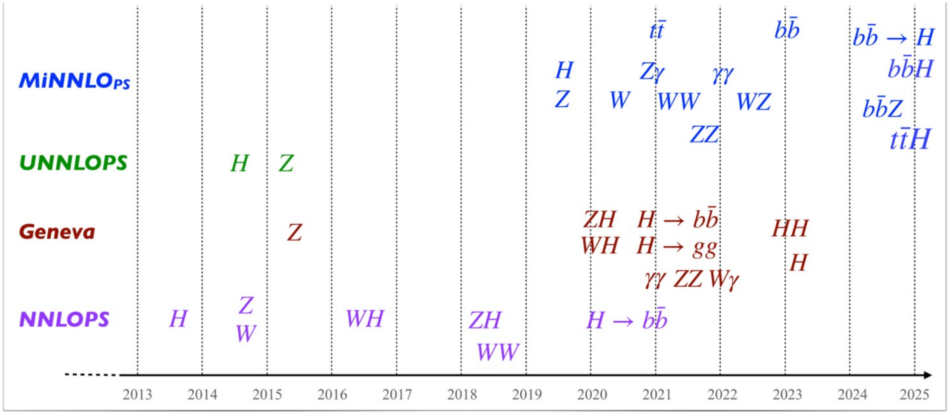
target to preserve LL accuracy so far

→ MiNNLOPS [Hamilton, Nason, Re, Zanderighi'13] [Monni, Nason, Re, Wiesemann, Zanderighi'20],

→ Geneva [Alioli, Bauer, Berggren, Hornig, Tackmann, Vermilion, Walsh, Zuberi'13-'25]

→ UN2LOPS [Hoche, Prestel'14]

→ Vincia [El-Menoufi,Preuss,Scyboz,Skands'24]



[talk by Wiesemann'25]

Other ideas to incorporate higher-orders:

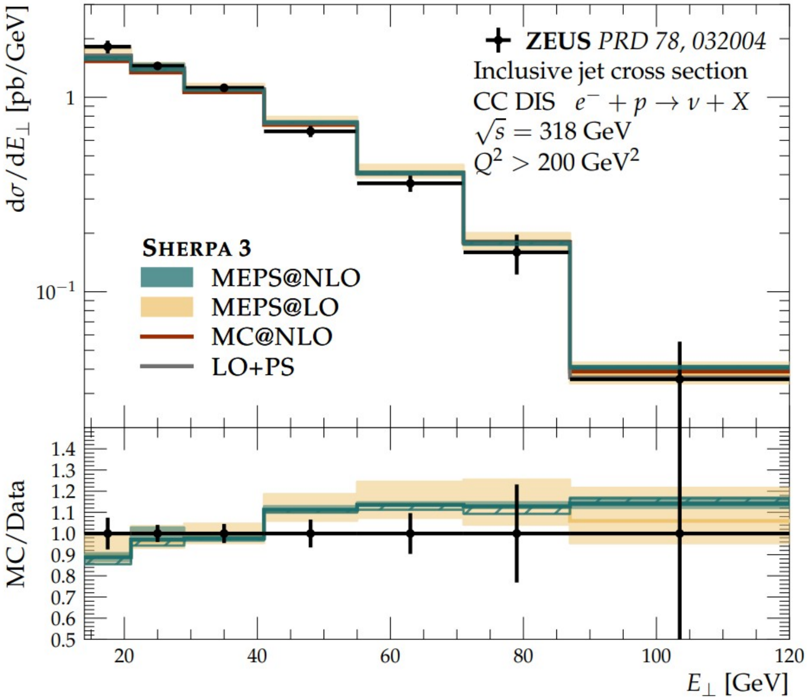
→ reweighting with energy-flow polynomials [Assi, Lee, Thaler'26]

NLO+PS for DIS

Conceptually pp frameworks capable of DIS processes
→ however requires **careful treatment of DIS kinematics** to be useful

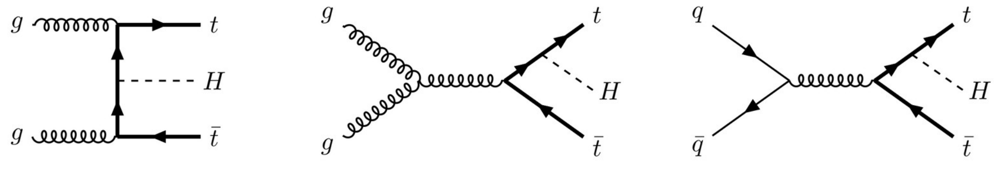
Recent works in MC Generators:

- Pythia: **Multi-Jet Merging/Production in Deep Inelastic Scatteringwith Pythia** [Helenius, Laulainen, Preuss'24] → **talk by Helenius**
- SHERPA: **Event generation at MEPS@NLO accuracy in neutral and charged current DIS at the EIC** [Meinzinger, Silvetti, Reichelt'25] → **talk by Reichelt**
- Powheg:
  → **A POWHEG generator for deep inelastic scattering**
  [Banfi, Ferrario Ravasio, Jäger, Karlberg, Reichenbach, Zanderighi'23]
  → **Parton-shower effects in polarized deep inelastic scattering**
  [Borsa, Jäger'24] → **talk by Borsa**
  → **An event generator for neutrino-induced deep inelastic scattering and applications to neutrino astronomy**
  [Ferrario Ravasio, Gauld, Jäger, Karlberg, Zanderighi'24]
  → **An event generator for Lepton-Hadron deep inelastic scattering at NLO+PS with POWHEG including mass effects**
  [Buonocore, Limatola, Nason, Tramontano'24]



NNLO PS with MiNNLOPS

Next-to-next-to-leading order event generation for $t\bar{t}H$ production with approximate two-loop amplitude
[Biello, Savoini, Signorile-Signorile, Wiesemann 2603.06143]
→ public event generator in Powheg framework



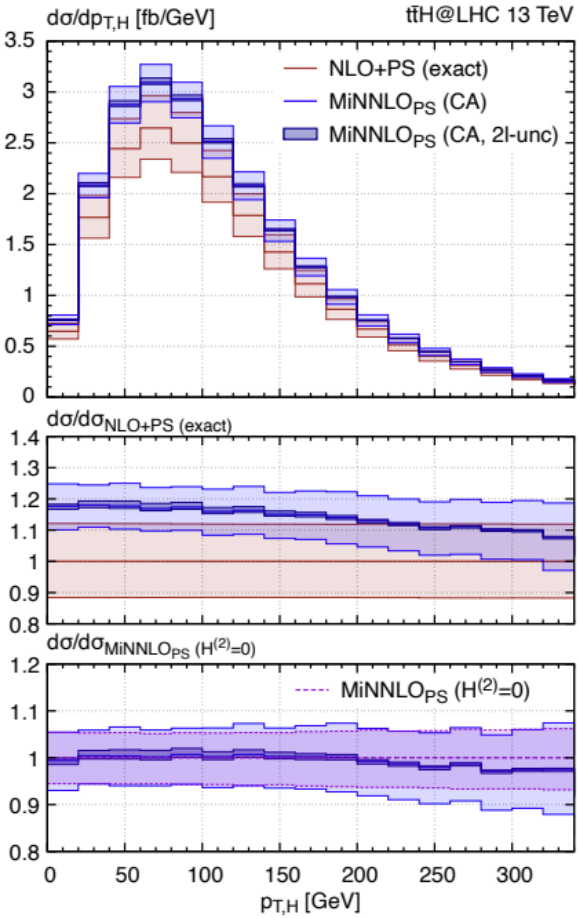
(a) t-channel gg diagram (b) s-channel gg diagram (c) s-channel $q\bar{q}$ diagram

Master formula:

$$d\sigma_{\mathrm{X}}^{\mathrm{MiNNLO_{PS}}} = d\Phi_{\mathrm{XJ}}\, \bar{B}^{\mathrm{MiNNLO_{PS}}} \times \left\{ \Delta_{\mathrm{pwg}}(\Lambda_{\mathrm{pwg}}) + d\Phi_{\mathrm{rad}} \Delta_{\mathrm{pwg}}(p_{\mathrm{T,rad}}) \frac{R_{\mathrm{XJ}}}{B_{\mathrm{XJ}}} \right\}$$

$$\bar{B}^{\mathrm{MiNNLO_{PS}}} \sim e^{-\tilde{S}(p_{\mathrm{T}})} \left\{ \frac{\alpha_s(p_{\mathrm{T}})}{2\pi} d\sigma_{\mathrm{XJ}}^{(1)} \left(1 + \frac{\alpha_s(p_{\mathrm{T}})}{2\pi} \tilde{S}^{(1)}(p_{\mathrm{T}})\right) + \left(\frac{\alpha_s(p_{\mathrm{T}})}{2\pi}\right)^2 d\sigma_{\mathrm{XJ}}^{(2)} + D^{(\geq 3)}(p_{\mathrm{T}}) \times F^{\mathrm{corr}} \right\}$$

approximate two-loop finite remainders based on soft-Higgs/massification approximations
→ few percent corrections to be expected



Local higher-order matching

Local NNLO matching Z → hadrons with Vincia

[El-Menoufi,Preuss,Scyboz,Skands'24]

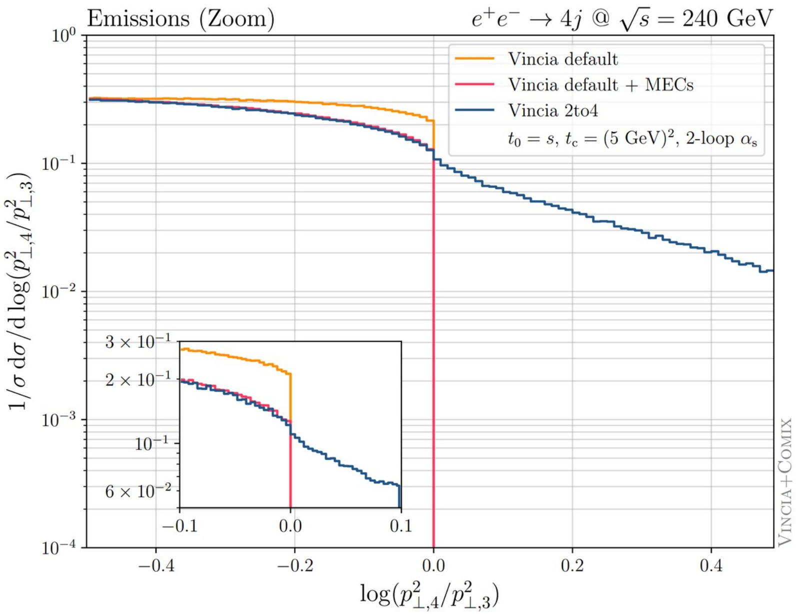
multiplicative matching:

'local NNLO k-factor'

$$
\begin{aligned}
\frac{m_Z}{8\pi^4}\frac{\mathrm{d}^2\Gamma}{\mathrm{d}\Phi_2} &= (\mathrm{B}_2+\mathrm{V}_2+\mathrm{W}_2) \\
&= \boxed{(\mathrm{B}_2+\mathrm{V}_2+\mathrm{W}_2)}\Big(\Delta_2(m_Z^2,t_c) \\
&\quad + \int \mathrm{d}\Phi_3\, \Delta_2(m_Z^2,t_3)\, A_{2\to3}\, \Delta_3(t_3,t_c)\, \delta^{(2)}(\Phi_2-\hat{\Phi}_2(\Phi_3)) \\
&\quad + \int \mathrm{d}\Phi_4\, \Theta(t_3-t_4)\, \Delta_2(m_Z^2,t_3)\, A_{2\to3}\, \Delta_3(t_3,t_4)\, A_{3\to4}\, \delta^{(2)}(\Phi_2-\hat{\Phi}_2(\Phi_4)) \\
&\quad + \int \mathrm{d}\Phi_4\, \Theta(t_4-t_3)\, \Delta_2(m_Z^2,t_4)\, A_{2\mapsto4}\, \delta^{(2)}(\Phi_2-\hat{\Phi}_2(\Phi_4))\Big) + \mathcal{O}(\alpha_s^3)\,,
\end{aligned}
$$

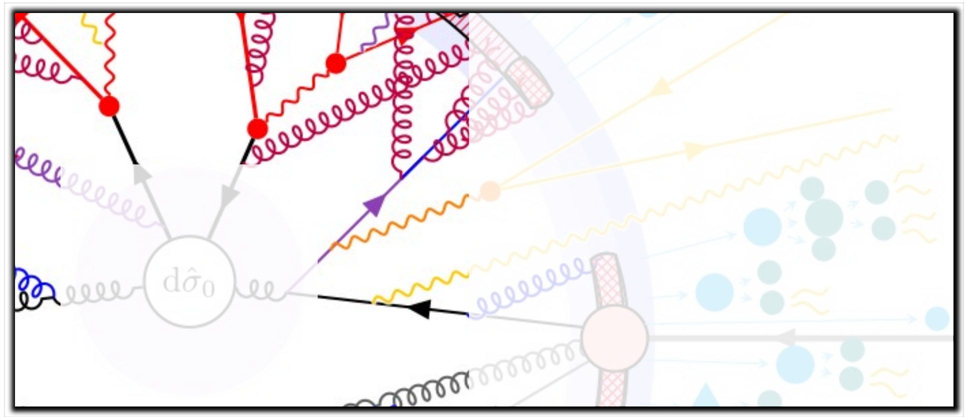
corrections to shower
→ ensure NLO for 3-jet to be correct (at leading color)
LO for 4-jet to be correct

Unordered 2→4 emissions:



[Campbell,Hoche,Li, Preuss,Skands'21]

Higher accuracy parton showers



Steps towards better controlled accuracy in the parton shower

→ **NLL showers**

→ **Sub-leading color effects**

Not covered here:

→ Higher-order splitting kernels

→ Treatment of spin-correlation [Hoeche, Hoppe, Reichelt'25]

→ Electroweak effects

Resummation in parton showers

Next-to-Leading Log (NLL) accuracy becomes the new standard:

PanScales

Logarithmic accuracy of parton showers: a fixed-order study - Dasgupta, Dreyer, Hamilton, Monni, Salam [1805.09327]
Parton showers beyond leading logarithmic accuracy - Dasgupta, Dreyer, Hamilton, Monni, Salam,Soyez [2002.11114]
Colour and logarithmic accuracy in final-state parton showers - Hamilton, Medves, Salam, Scyboz, Soyez[2011.10054]
Spin correlations in final-state partonshowers and jet observables - Karlberg, Salam, Scyboz, Verheyen [2103.16526]
Soft spin correlations in final-state parton showers - Hamilton, Karlberg, Salam, Scyboz, Verheyen [2111.01161]
PanScales parton showers for hadron collisions: formulation and fixed-order studies - van Beekveld, Ferrario Ravasio, Salam, Soto Ontoso, Soyez, Verheyen [2205.02237]
PanScales parton showers for hadron collisions: all-order validation- van Beekveld, Ferrario Ravasio, Hamilton, Salam, Soto Ontoso, Soyez, Verheyen [2207.09467]
Next-to-leading-logarithmic PanScales showers for deep inelastic scattering and vector boson fusion - van Beekveld, Ferrario Ravasio [2305.08645]

Alaric

A new approach to color-coherent parton evolution - Herren, Höche, Krauss, Reichelt, Schönherr [2208.06057]
New approach to QCD nal-state evolution in processes with massive partons - Assi, Höche [2307.00728]
The Alaric parton shower for hadron colliders - Höche, Krauss, Reichelt [2404.14360]

Apollo

A partitioned dipole-antenna shower with improved transverse recoil - Preuss [2403.19452]

Deductor

Summation of large logarithms by parton showers - Nagy, Soper [2011.04773]
Summation by parton showers of large logarithms in electron-positron annihilation - Nagy, Soper [2011.04777]

Herwig

Building a consistent parton shower - Forshaw, Holguin, Plätzer [2003.06400]
Improvements on dipole shower colour - Forshaw, Holguin, Plätzer [2011.15087]
Logarithmic accuracy of angular-ordered parton showers - Bewick, Ferrario Ravasio, Richardson, Seymour [1904.11866]
Initial state radiation in the Herwig 7 angular-ordered parton shower - Bewick, Ferrario Ravasio, Richardson, Seymour [2107.04051]

Next step: confrontation of these showers with phenomenology

Jet substructure: where logarithmic accuracy matters

Jet sub-structure

- Example: Lund plane multiplicity by ATLAS
- comparison of different showers and analytic resummed predictions
- Data is sensitive to the shower model
  → how to estimate shower uncertainties?
  → why are the shower so different from the analytic resummation?

Outlook

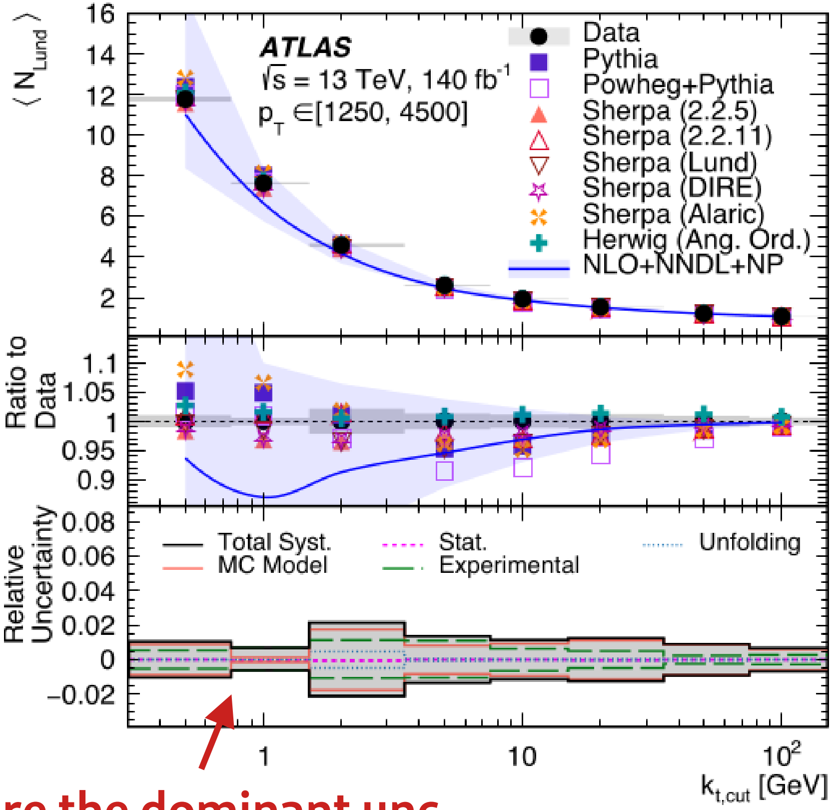
→ Implications for jet substructure measurements

→ everything that uses jet substructure techniques

→ flavour tagging

→ quark/gluon jet discrimination

→ jet calibration



MCs are the dominant unc.

Towards NNLL showers

- For some e+e- event shapes already feasible

→ PanScales showers + Pythia

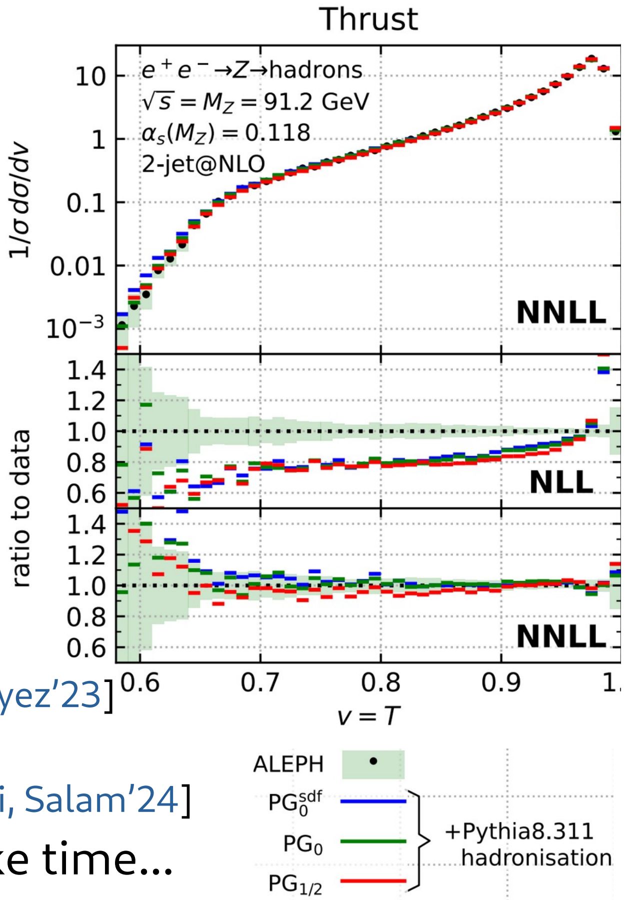
→ understood with $\alpha_S = 0.118$ at NLL → NNLL spot on

→ other showers might behave differently

- Take-home message:

→ high log accuracy can resolves modelling issues

→ increased consistency



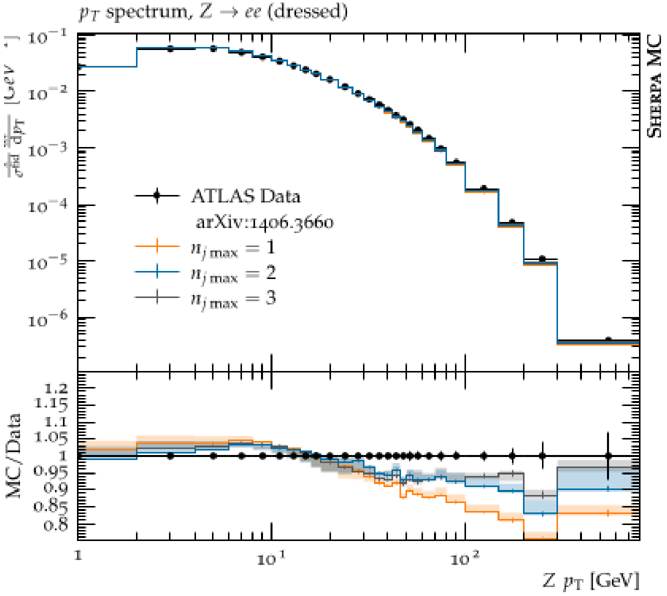
Step-by-step towards NNLL showers come up

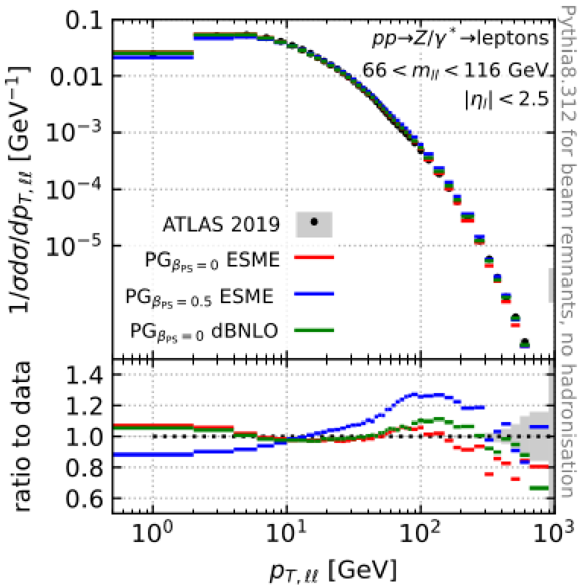
- Double soft-corrections [Ferrario Ravasio, Hamliton, Karlberg, Salam, Scyboz, Soyez'23]
- Soft-collinear emissions [PanScales'24]
- Triple-collinear emissions [van Beekveld, Dasgupta, el-Menoufi, Helliwell, Monni, Salam'24]

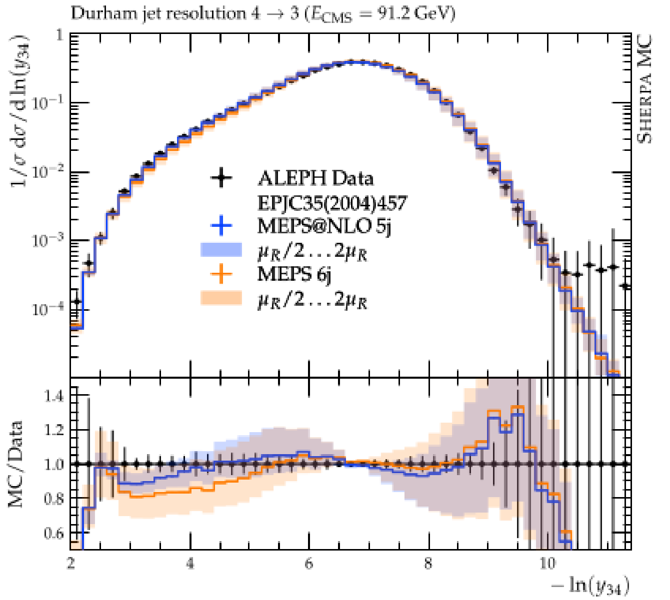
→ so far limited to special cases in e+e-, transfer to pp/DIS will take time...

Matching and merging of NLL showers

Examples (plots from left-to-right):
- Alaric LO merging in Z+jets [Hoeche, Krauss, Reichelt'24]
- PanScales NLO for DY [PanScales'25]
- Alaric NLO merging at LEP [Hoeche, Krauss, Meinzinger, Reichelt'25]



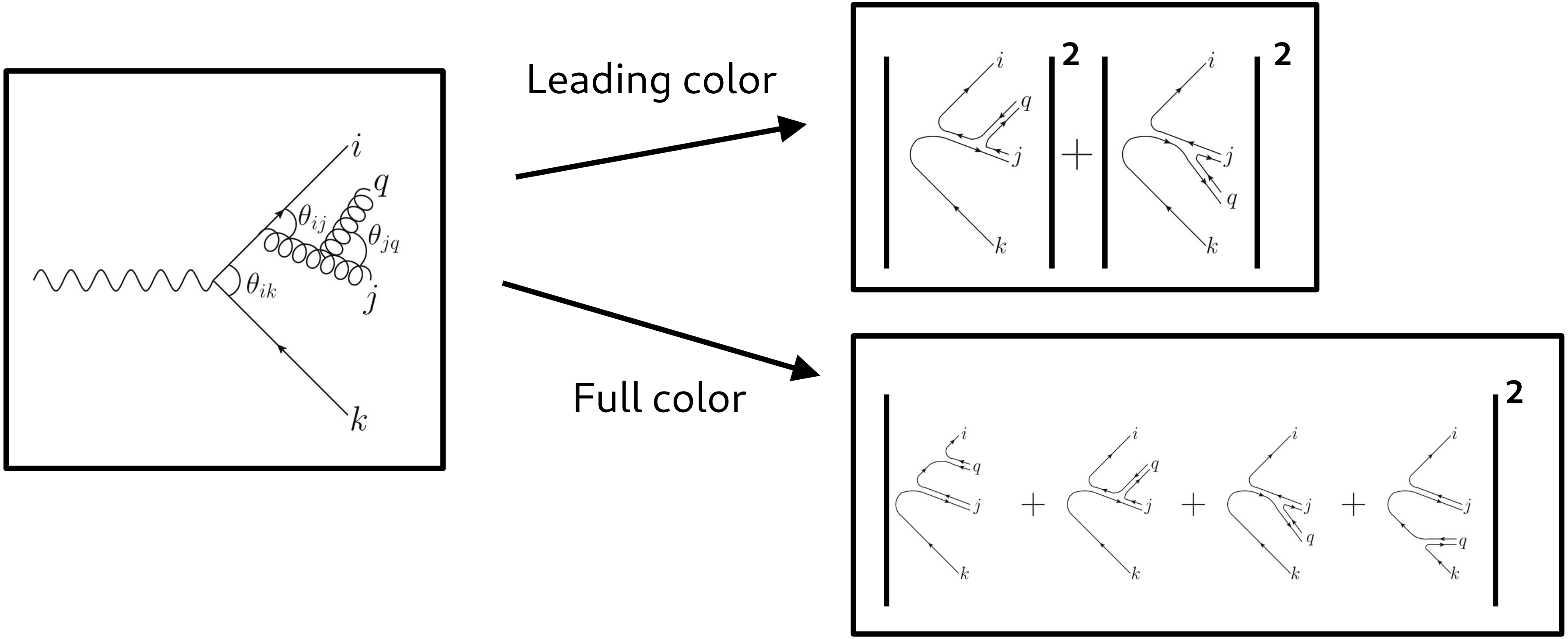




Sub-leading color evolution

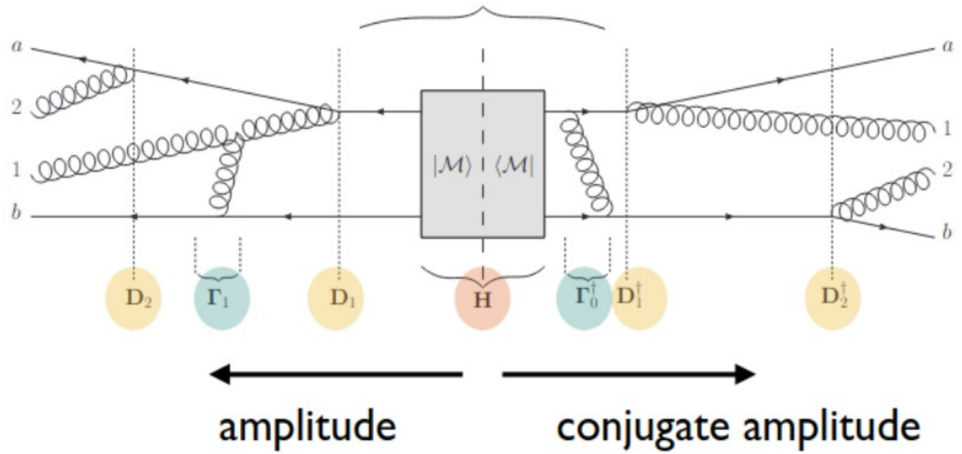
[Diagrams from Holguin, Forshaw, Plaetzer'21]

Most showers work in leading color approximation: $N_c \to \infty$

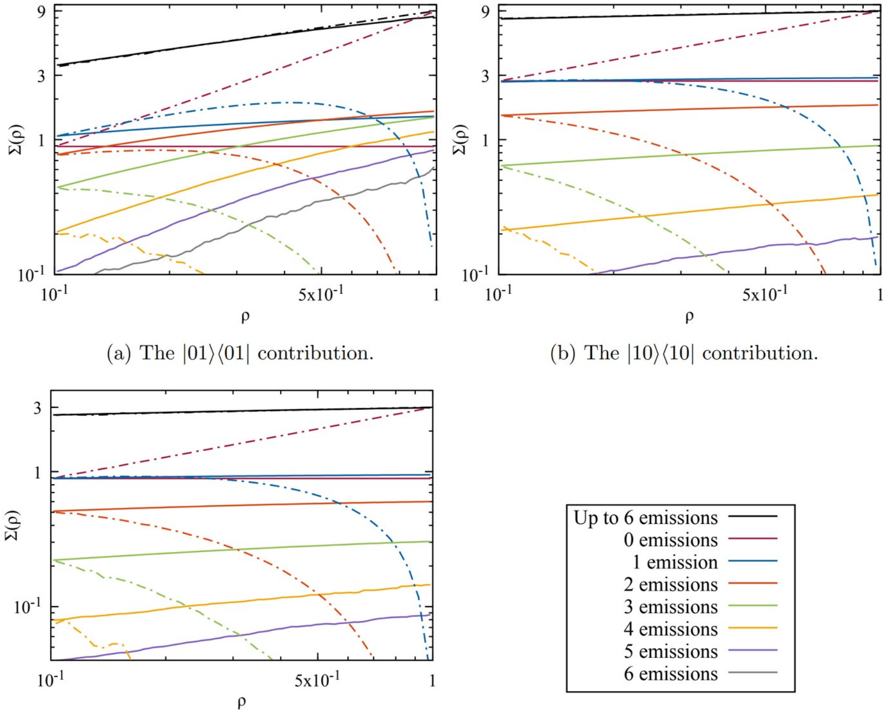


Sub-leading color evolution

In general events have complicated color structure:



[Forshaw, Plaetzer, Torre'25]



(a) The $|01\rangle\langle 01|$ contribution.

(b) The $|10\rangle\langle 10|$ contribution.

(c) The $|10\rangle\langle 01|$ (interference) contribution.

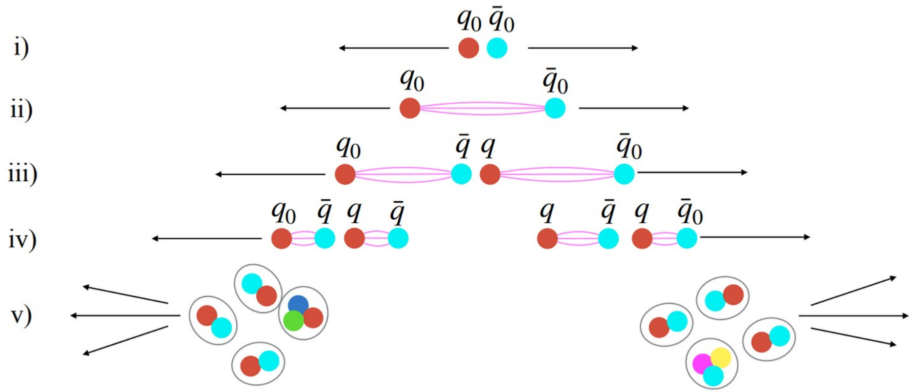
Methods implementing sub-leading color evolution

- subleading color effects in soft gluon emissions [Hatta, Ueda'13'20]
- Deductor [Nagy, Soper'07-15]
- Cvolver [De Angelis, Forshaw, Holguin, Plaetzer, Torre,'13-'25]

Hadronization

String Model (Pythia)

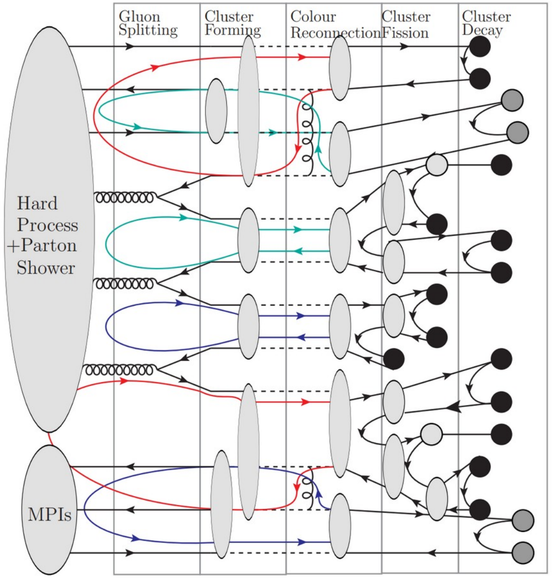
→ dynamics of a 1d color field (string)



[pic from Altmann, Bernardinis, Skands, Zaccolo'25]

The Cluster Model (Herwig/Sherpa)

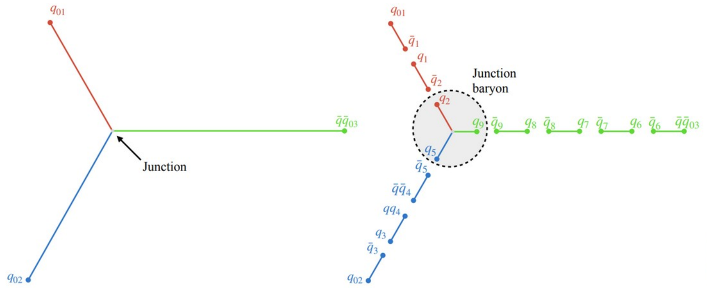
→ partons form color-singlet clusters which decay to hadrons

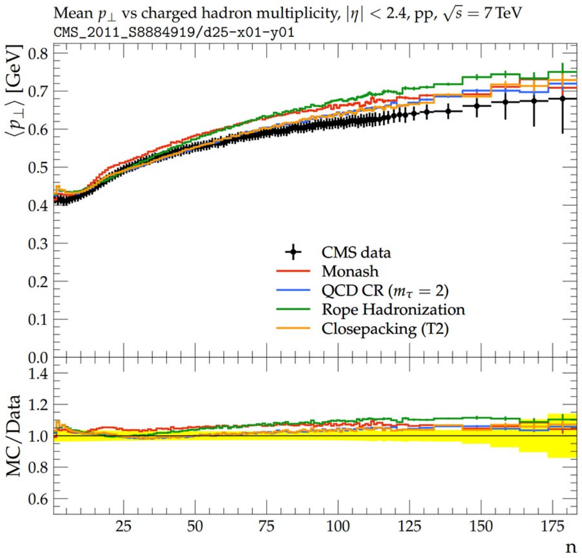


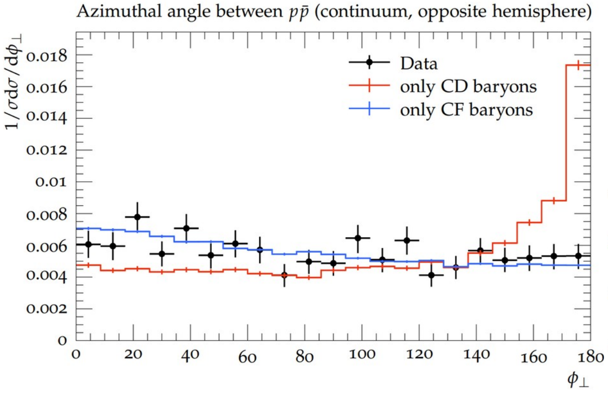
[Herwig 7]

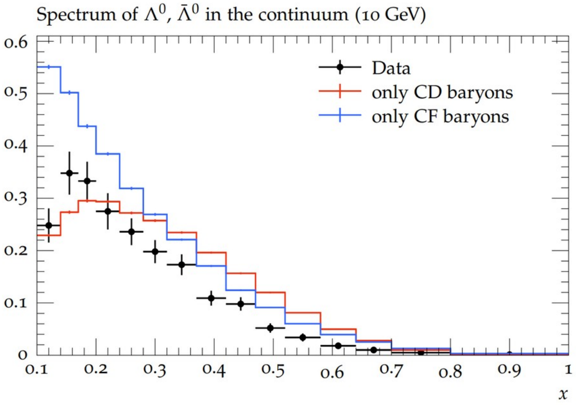
Hadronization – new developments

New developments Closepacking effects on strangeness and baryon production at the LHC
[Altmann, Bernardinis, Skands, Zaccolo'25]







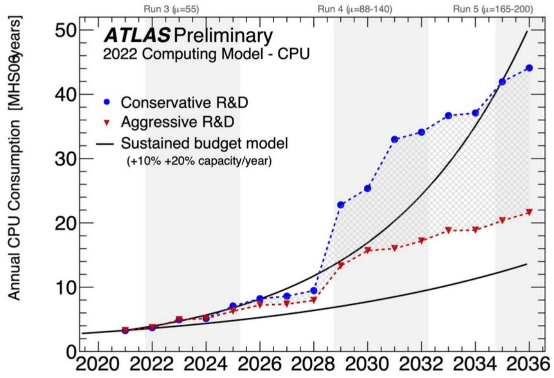


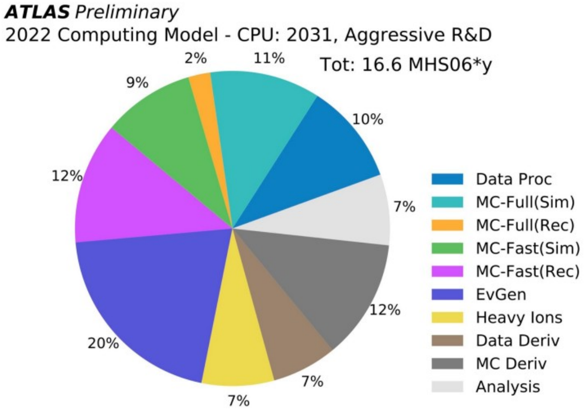
Phenomenological constraints of the building blocks of the cluster hadronization model
[Gieseke, Kiebacher, Plaetzer, Priedigkeit'25]

Computational challenges

The HL-LHC Problem
Generating enough events is/will be computationally expensive
1) **negative events**
2) **expensive higher point ME unweighting**

[CERN-LHCC-2022-005]





Ensure positivity of event weights

- Positive matching: ESME [PanScales'25], KrK [Pratixan, Siodmok, Whitehead '24]
- Reweighting methods: cell-resampling [J. Andersen, A. Maier'21+Maître'23]
  Arcane [Shyamsundar'25]

Exploit modern architectures → CPU + GPU

- MEs: PEPPER [Bothmann, Childers, Giele, Höche, Isaacson Knobbe'23]
- Madgraph on GPUs [Valassi, Childers, Hageböck, Massaro, Mattelaer, Nichols, Optolowicz, Roiser, Teig, Wettersten'25]

Machine Learning Methods

- Neural Importance Sampling
- Surrogates to emulating MEs

Neural importance sampling & surrogates

Variance reduction through importance sampling:

$$\hat{I} = \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i)\,, \quad \delta\hat{I} = \sqrt{\frac{1}{N-1}\left(\frac{1}{N}\sum_{i=1}^{N} f^2(\mathbf{x}_i) - \hat{I}^2\right)}$$

$$I = \int_{\mathbf{H}(\mathbf{x})\in\Omega} \mathrm{d}\mathbf{H}\,\frac{f(\mathbf{x})}{h(\mathbf{x})} \qquad h(\mathbf{x}) = \left|\det\left(\frac{\partial\mathbf{H}(\mathbf{x})}{\partial\mathbf{x}}\right)\right|$$

Task: find $h(\mathbf{x})$adaptive MC techniques: VEGAS [Lepage'78], Parni [Hameren'14]

Neural importance sampling

Normalising Flows in Sherpa [Bothmann'20], Madgraph [Heimel'22'25],STRIPPER [Jansen'25]

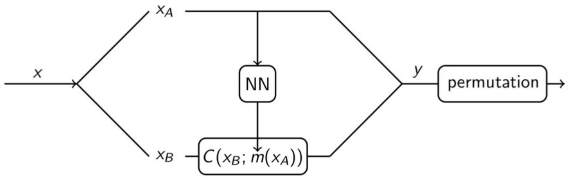
Surrogates

If f(x) is very expensive → finding a surrogate improves performance
→ can be unbiased by unweighting against real f(x)

- QCD factorization aware NN ME emulators [Maitre'21] [Janssen'23]
- two-stage unweighting to correct surrogates [Danziger'22]
- one-loop emulators [Aylett-Bullock'21][Badger'23] [Maitre'23]

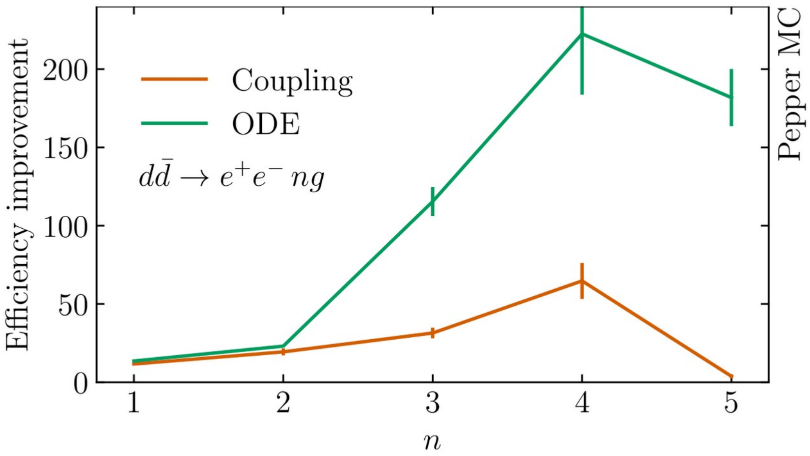
Unweighting with Normalizing Flows

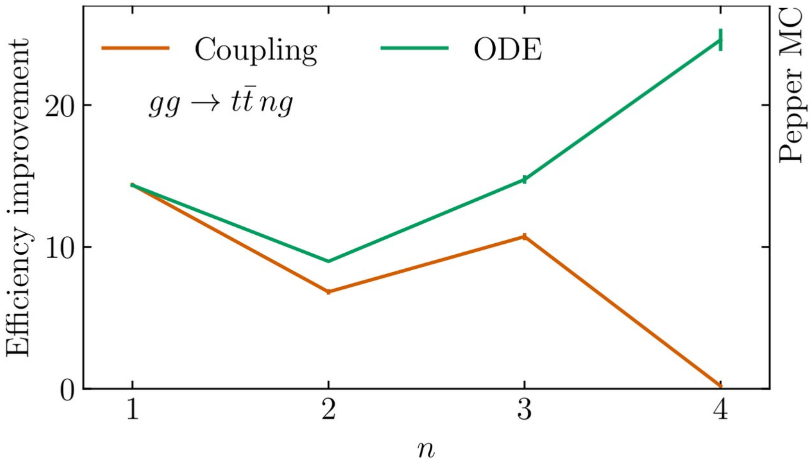
Coupling Layer Flows → series of simple bijections



Continuos Normalising Flows $\frac{\mathrm{d}\psi_t(x)}{\mathrm{d}t} = v_t(\psi_t(x))$

Substantial unweighting efficiency improvements $\epsilon_\theta = \frac{\langle w_\theta \rangle}{w_{\max,\theta}} \quad \text{with} \quad w_\theta(x) := \frac{p_0(x)}{q_\theta(x)}.$



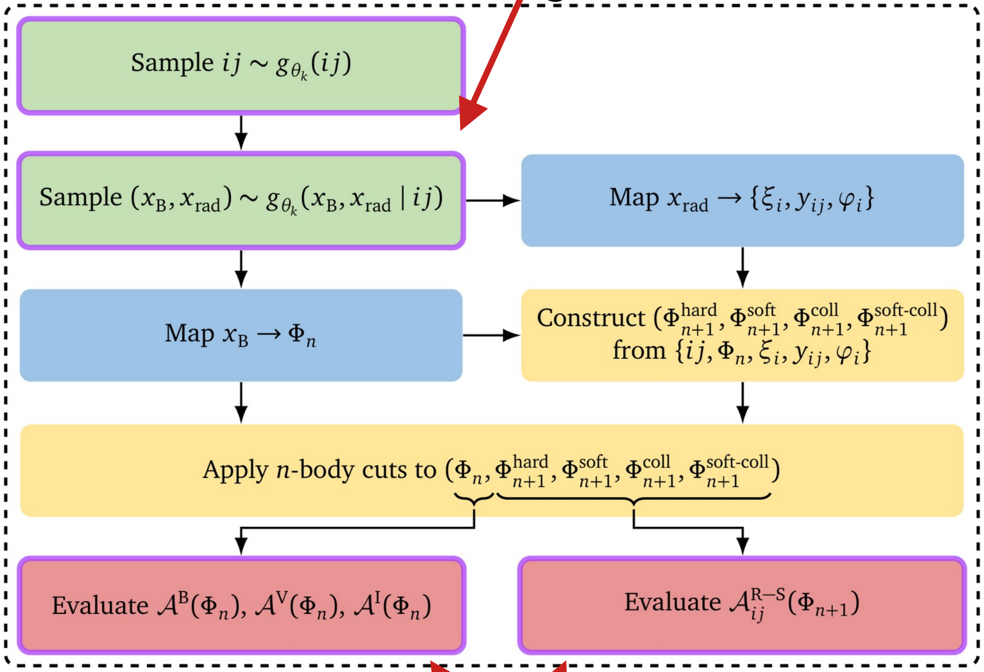


[Bothmann, Janßen, Knobbe, Schmitzer, Sinz, 2604.03511]

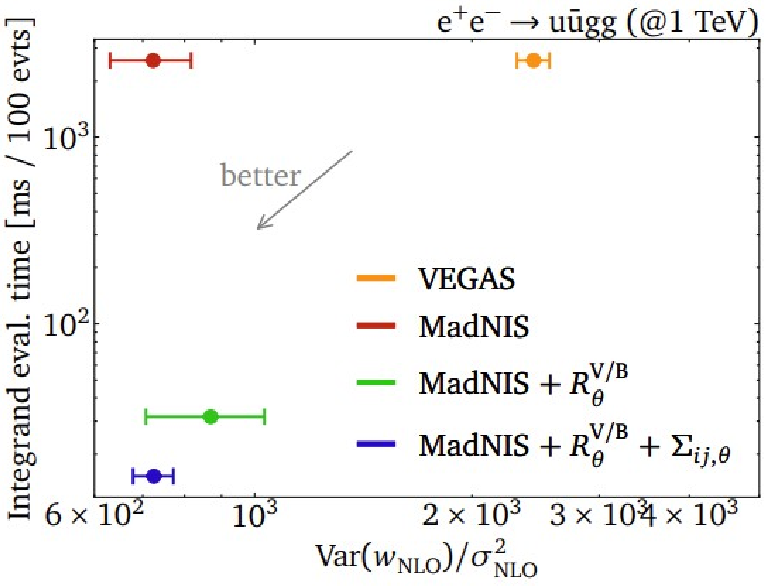
Surrogates + Normalising flows

Madnis@NLO [De Crescenzo, Mariño, Elmer, Heimel, Plehn, Winterhalder, Zaro 2603.22407]

Normalizing Flows



Surrogates



Summary and Outlook

- MC Generators for hadron collisions have evolved in the last decades from **"order-of-magnitude"** tools to **precision instruments**.
- **NNLO+PS** and **NLL showers** are the new standard for the 2020s.
- Success of the LHC physics program **depends on the continued evolution** of these tools.
- Challenges = Outlook:
  - Generalizations of new developments to arbitrary processes
    → beyond NNLL, (local) NNLO+PS matching, sub-leading color
  - QCDxEW mixed for precision observables (Drell-Yan for example)
  - Performance bottlenecks: negative weights, hybrid architectures