# Novel Concepts and Methodology for Simulation in High-Energy Physics

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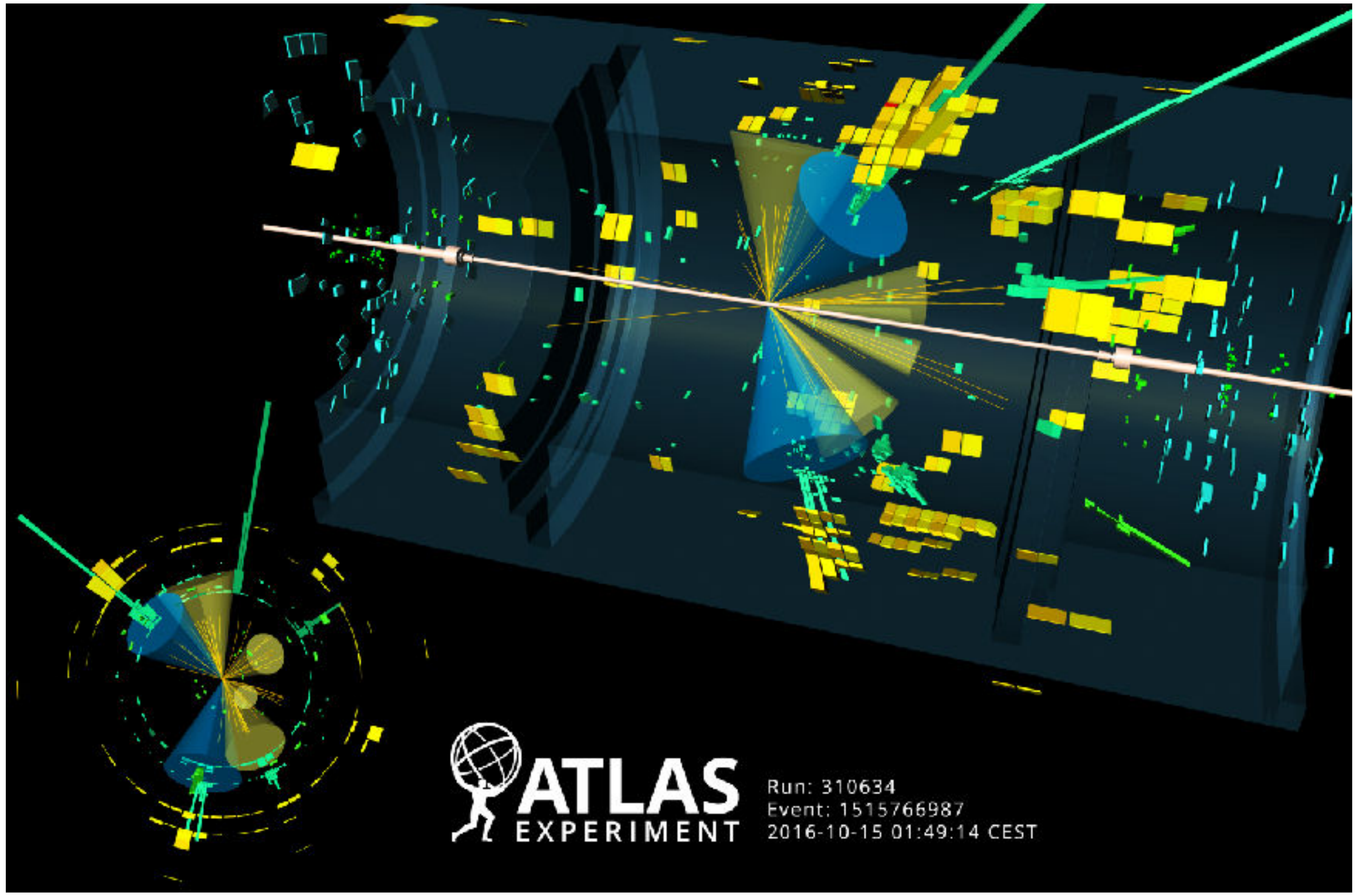
# The Challenge of Complexity

**Collider experiments** have established the Standard Model of Particle Physics — which we know is incomplete.

Shortcomings of the Standard Model must reveal as tiny deviations from the rich dynamics at colliders.

The challenge is to predict the properties of these final states **accurately and precisely,** to compare to increasingly precise measurements.

Detailed predictions call for **algorithmic approaches and (Monte Carlo) simulation.**



# QCD and the role of event simulation

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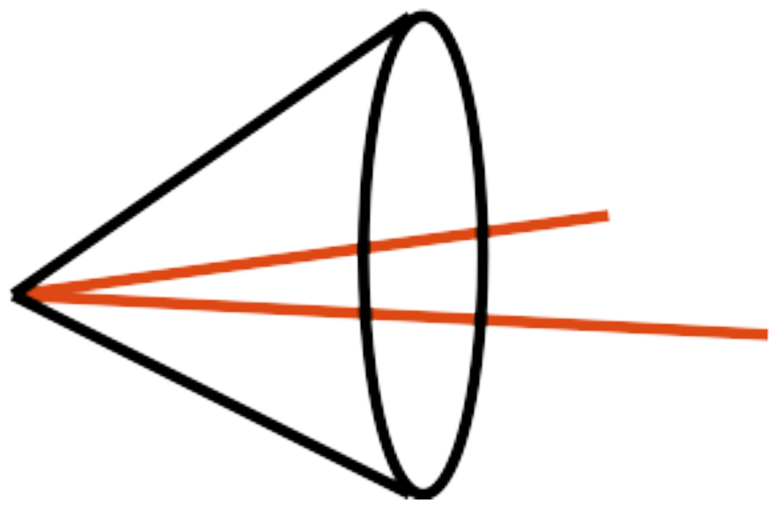
**Strong interactions** are the main source of the complexity and the rich phenomenology. QCD describes the dynamics of quarks and gluons bound in hadrons.

Perturbative calculations are possible at short time scales:
Strong coupling is large only at small energy scales.

$$\alpha_s(100\ \mathrm{GeV}) \approx 0.117$$

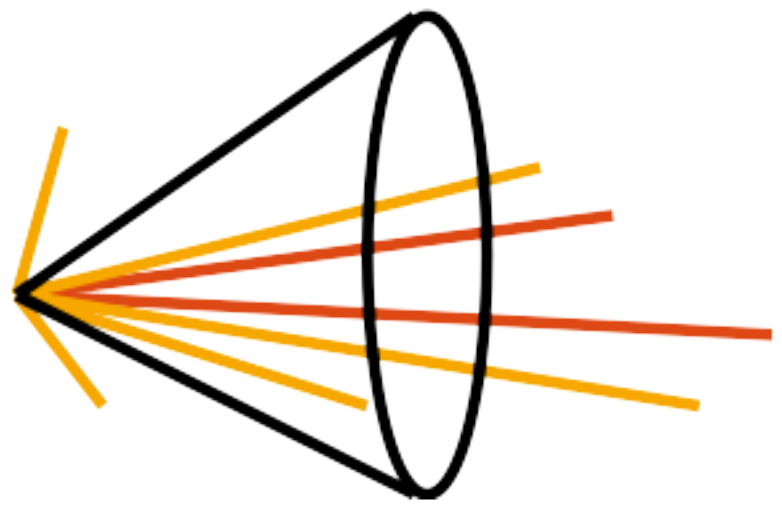
Fixed order **theory**:
**partonic** cross section.

~ 10% precise,
steadily improving



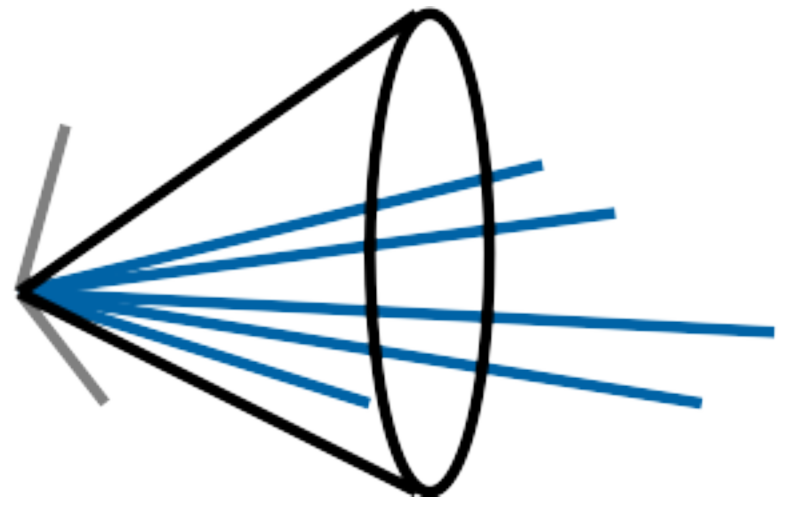
**Event generator:**
**Evolution** into jets.

Leading corrections to all orders,
**accuracy mostly unclear**



**Experiment:**
**Hadronic** final state.

**1% precision in reach,**
sophisticated algorithms.

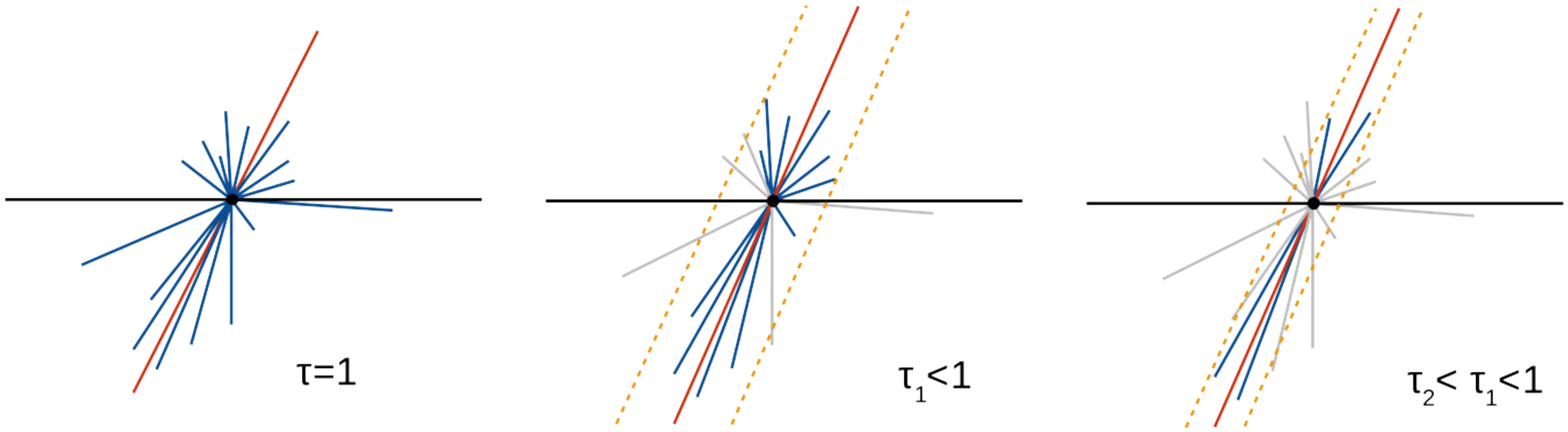


# QCD and the role of event simulation

**Strong interactions** are the main source of the complexity and the rich phenomenology. QCD describes the dynamics of quarks and gluons bound in hadrons.

Resummation is needed if large logarithms overcome the small coupling.

$$\sigma(n \text{ jets}, \tau) \sim \sum_k \sum_{l \leq 2k} c_{nkl} \; \alpha_s^k(Q) \; \ln^l \frac{1}{\tau}$$




**Invert the jet evolution** to map hadronic configurations to partonic final states.
Observables involve resolution parameter: Limit radiation at certain momentum scales.

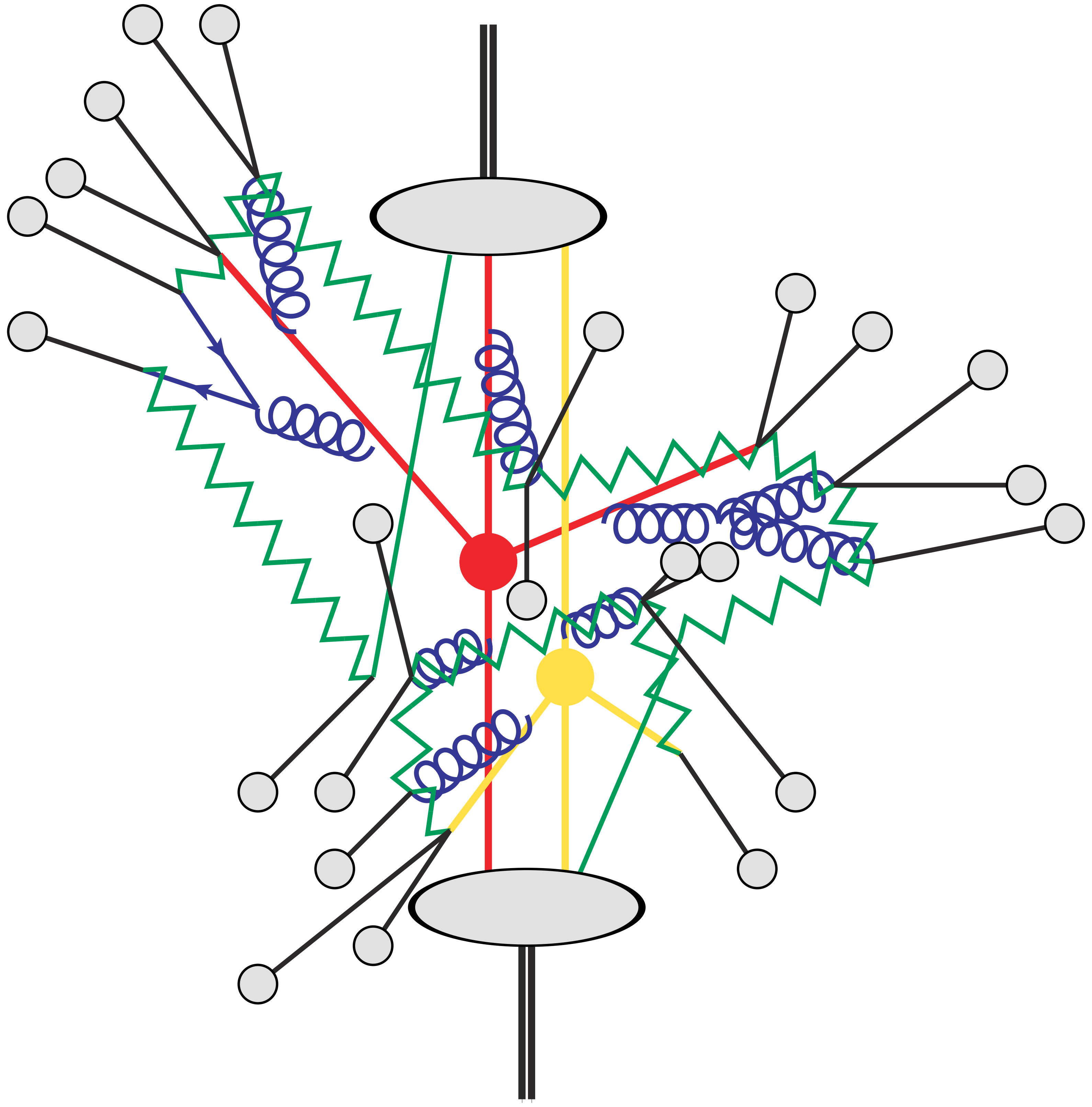
# Complexity Factorized

Hierarchy of energy scales allows for factorisation:

Hard partonic scattering
Jet evolution
Multi-parton interactions
Hadronization

**Analytic approaches:**
Accurate for specific class of observables.

**Event generators:**
Universal, but lack a systematic expansion.



$$d\sigma \sim d\sigma_{\mathrm{hard}}(Q) \times \mathrm{PS}(Q \to \mu) \times \mathrm{Had}(\mu \to \Lambda)$$

# Complexity Factorized



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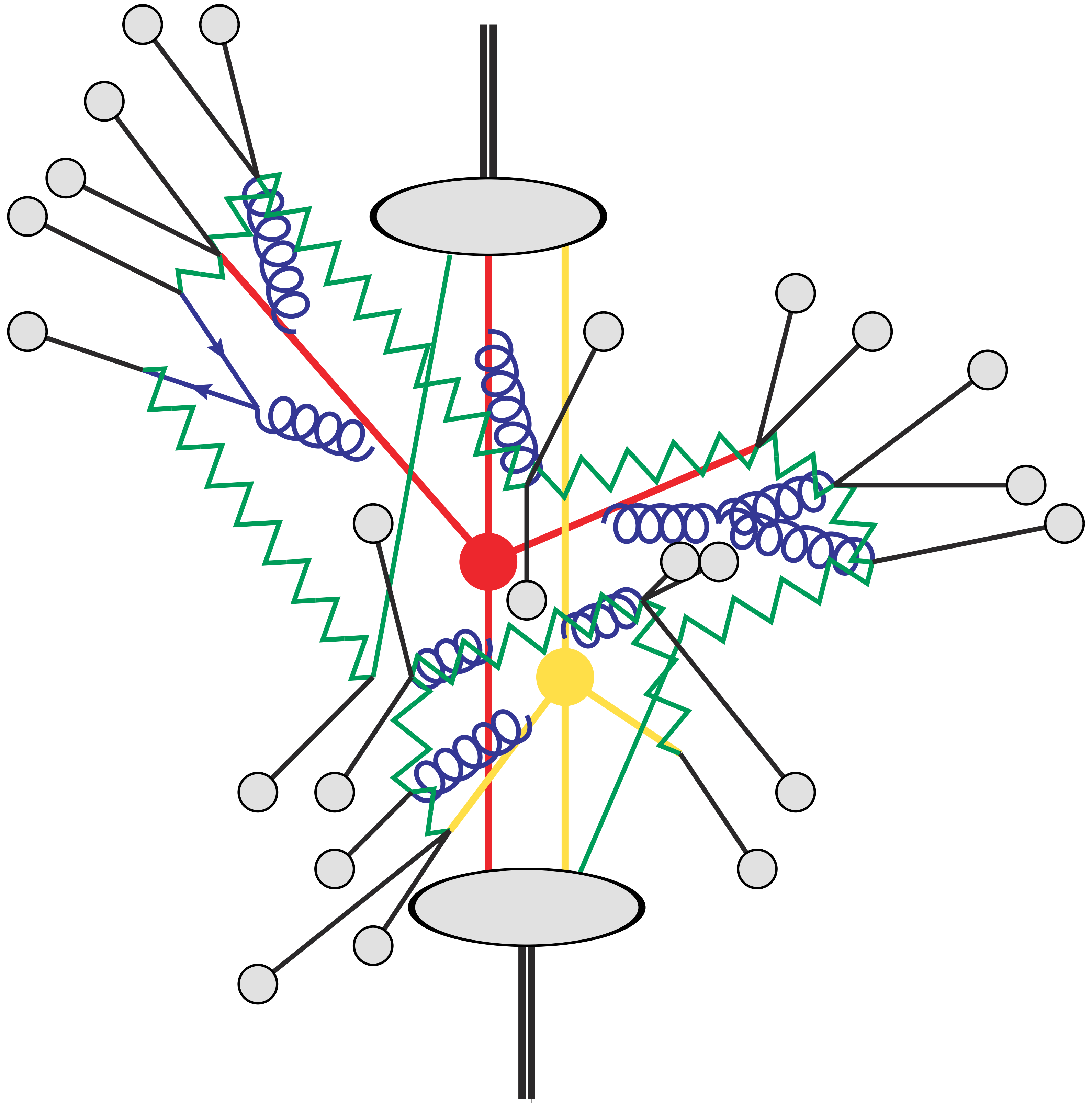


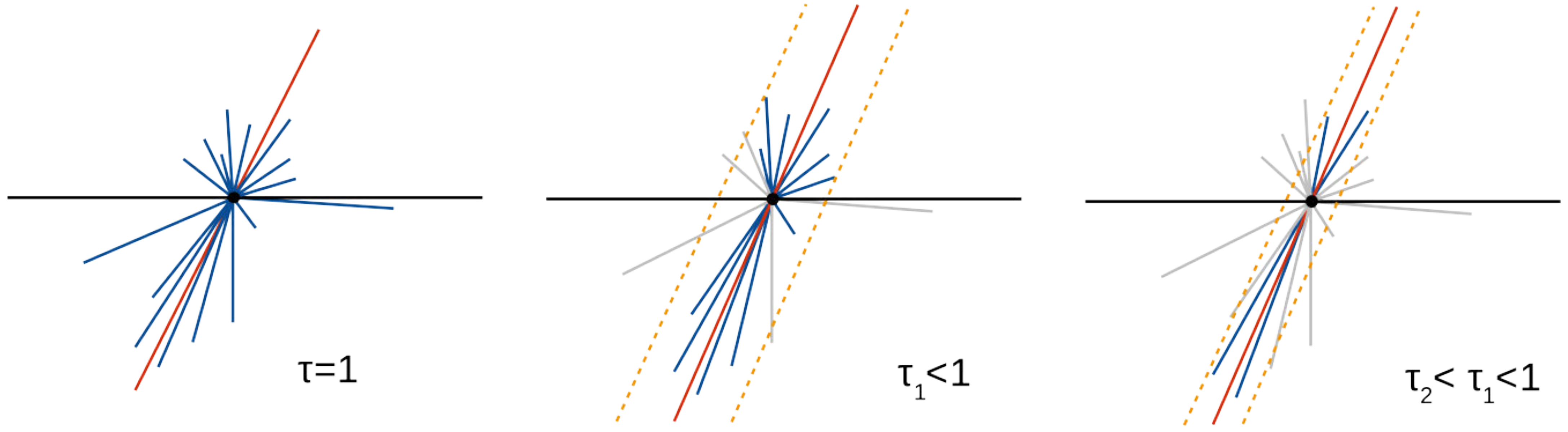
Precise QCD predictions need to incorporate **corrections to the hard process** and **improved parton evolution**, addressing analytic applications and simulation.

Interplay with models of soft QCD is crucial.

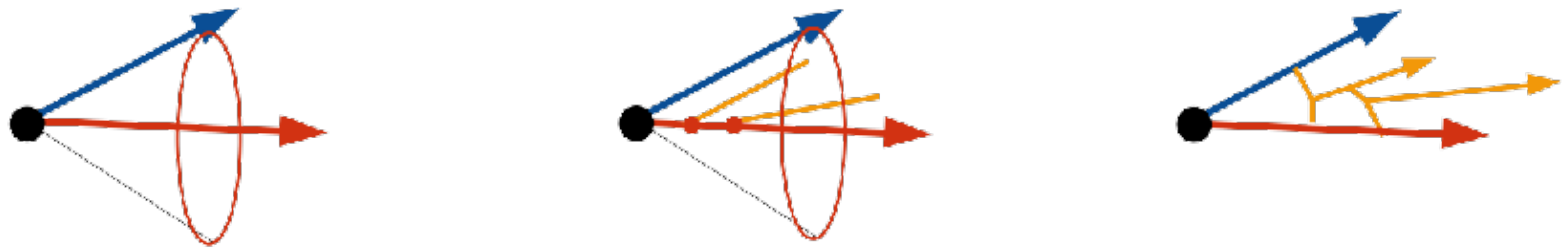
$$\mathrm{d}\sigma \sim \mathrm{d}\sigma_{\mathrm{hard}}(Q) \times \mathrm{PS}(Q \to \mu) \times \mathrm{Had}(\mu \to \Lambda)$$

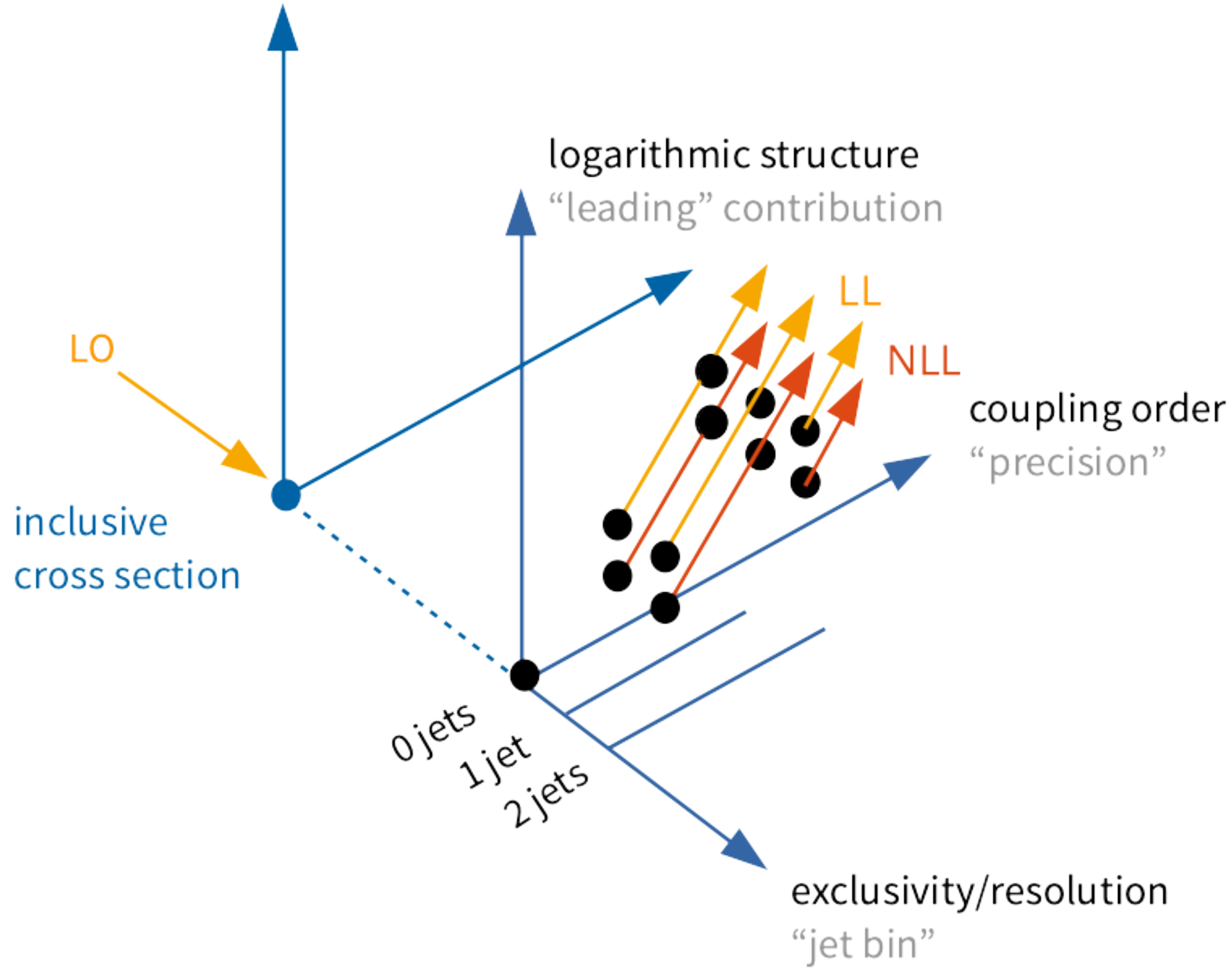
# State of the art: Jets & NLO Corrections

$$\sigma(n \text{ jets}, \tau) \sim \sum_k \sum_{l \leq 2k} c_{nkl}\, \alpha_s^k(Q)\, \ln^l \frac{1}{\tau}$$




Global deviations from jets governed by QCD coherence




[Catani, Trentadue, Marchesini, Webber, …]

recent application to heavy quarks [Hoang, Plätzer, Samitz — JHEP 1810 (2018) 200]

# State of the art: Jets & NLO Corrections

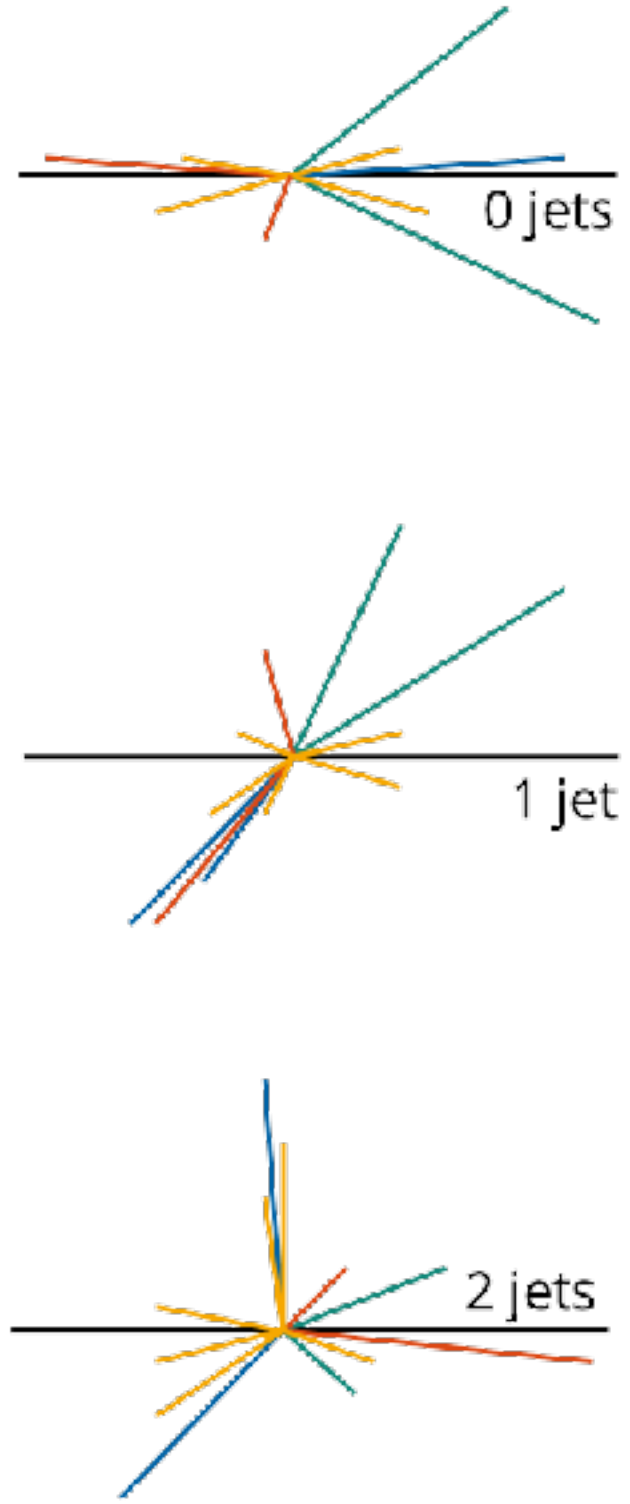
$$\sigma(n \text{ jets}, \tau) \sim \sum_k \sum_{l \leq 2k} c_{nkl}\ \alpha_s^k(Q)\ \ln^l \frac{1}{\tau}$$

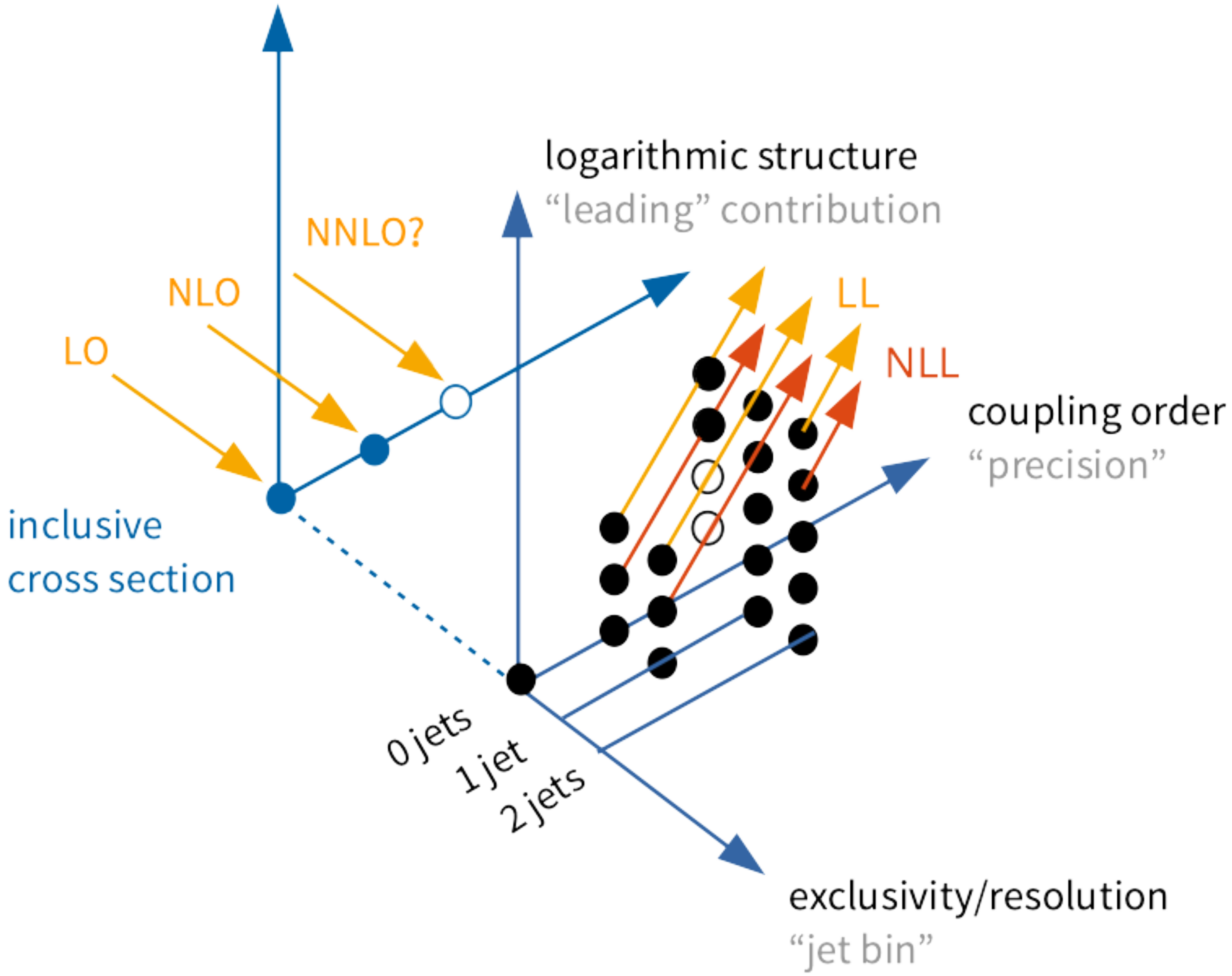
Matching to NLO is established, basis of combining jet multiplicities.

Need for unitarization is a consequence of the lowest order approximation adopted for the shower.

[Plätzer — JHEP 08 (2013) 114]
[Lönnblad, Prestel — JHEP 02 (2013) 049]
MI(N)NLO approaches [Hamilton, Nason, Zanderighi, …]

Can combine with NNLO for some processes, but not as universal as established for NLO.



# State of the art: The Herwig 7 Event Generator

[Herwig(++) collaboration – EPJ C58 (2008) 639 + release notes]
[Herwig collaboration – EPJ C76 (2016) 665 + release notes]


Herwig is one of the most used multipurpose event generators, with emphasis on perturbative QCD: Precise predictions have naturally become our target.

The theoretical insight into matching and merging required an automated and highly flexible module for doing NLO QCD calculations: **Matchbox.**

[Plätzer –- with Bellm, Wilcock, Rauch, Reuschle, 2011 – 2015]
preliminary results in [Plätzer, Gieseke – EPJ C72 (2012) 2187]

**Two shower algorithms** and two matching schemes allow to cross check predictions in lack of a more systematic way of evaluating uncertainties.

[Gieseke, Stephens, Webber – JHEP 0312 (2003) 045]
[Plätzer, Gieseke – JHEP 1101 (2011) 024]
[Bellm, Nail, Plätzer, Schichtel, Siodmok – EPJ C76 (2016) 665]

[Plätzer — JHEP 1308 (2013) 114]
[Bellm, Gieseke, Plätzer — EPJ C78 (2018) 244]

Automated **NLO matching and multi jet merging.**

# Phenomenology at the LHC and beyond

VBSCan
LHC Higgs Working Group
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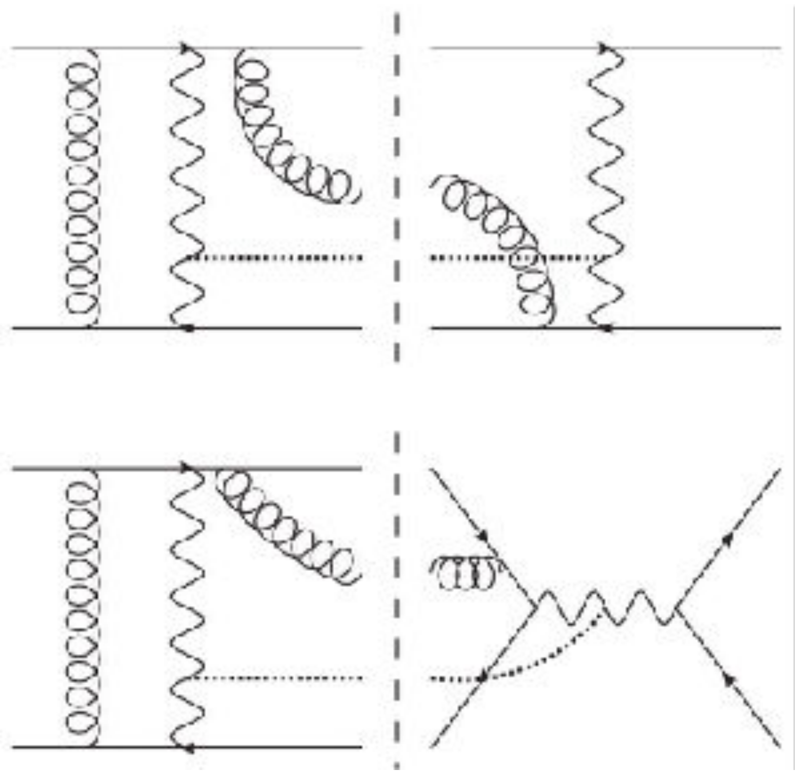
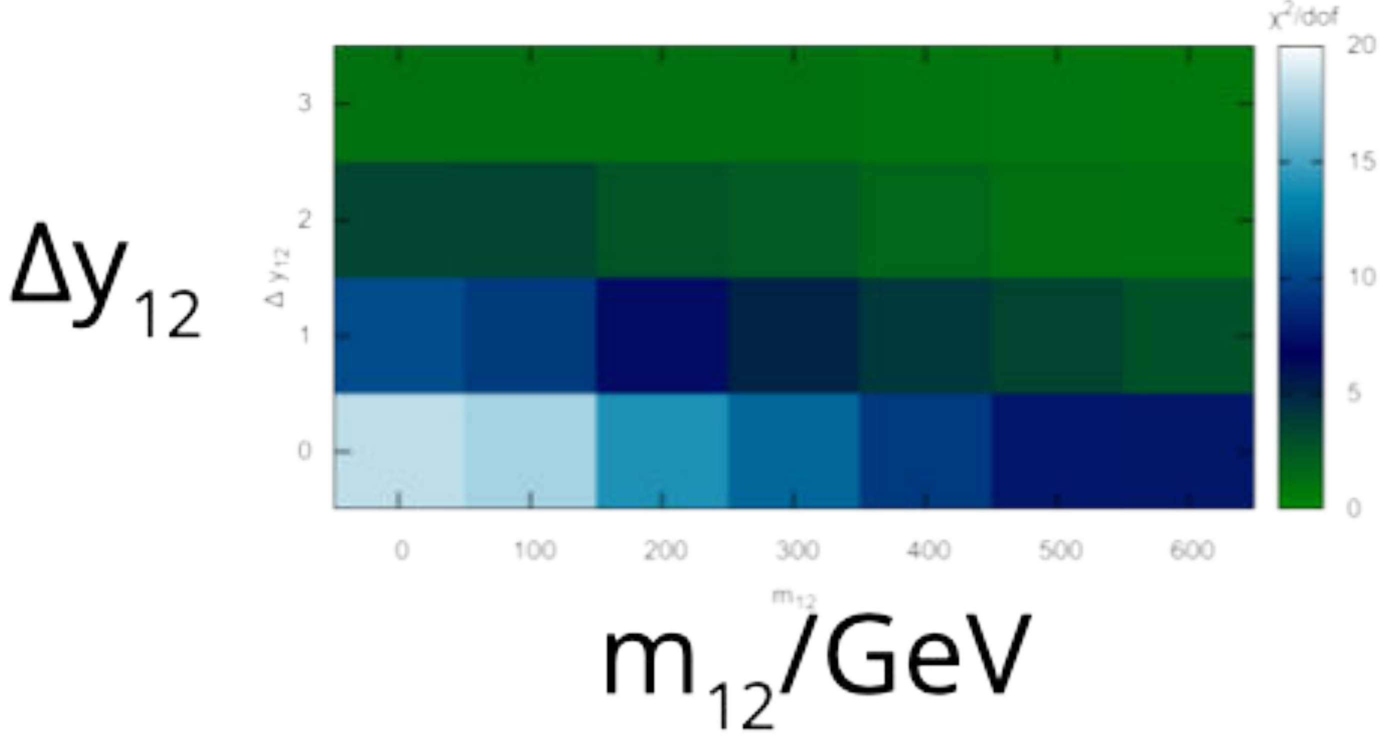
Current focus is on processes of interest to the past and future LHC runs.
Specifically important: **Vector Boson Fusion** and Vector Boson Scattering.


Full NLO QCD corrections to electroweak H+2,3 jet production.



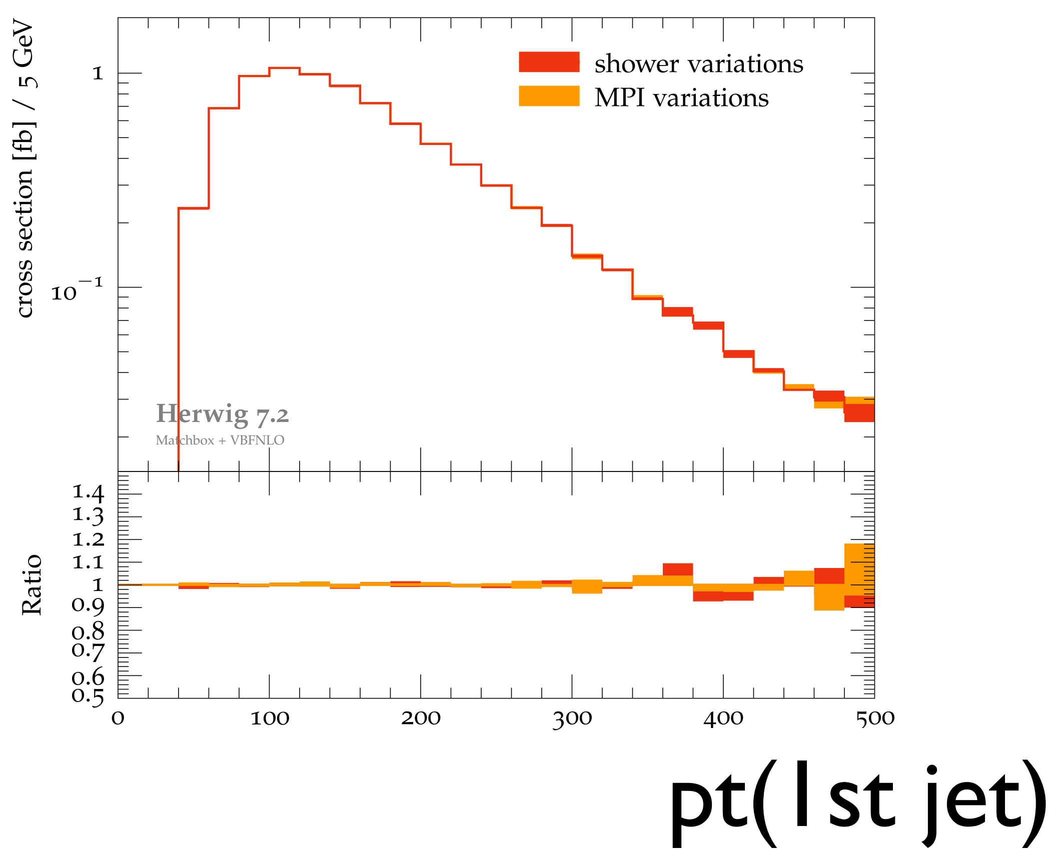


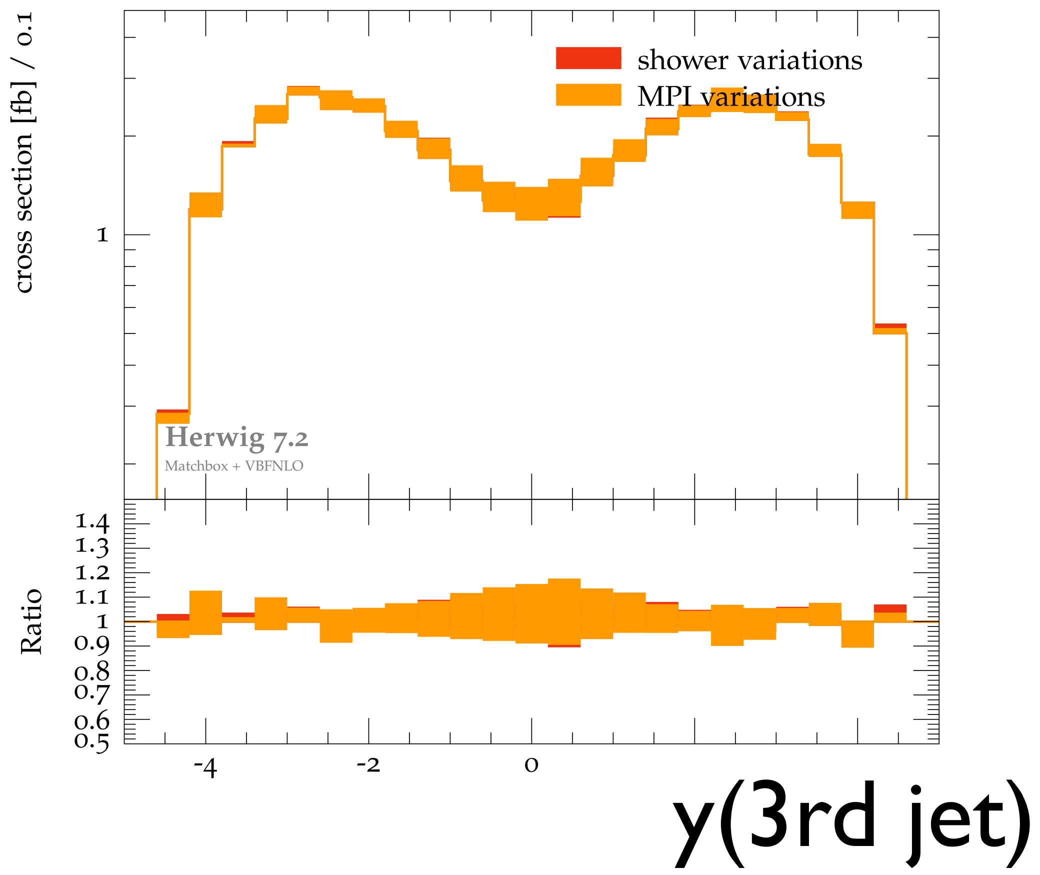

[Campanario, Figy, Plätzer, Sjödahl – PRL 111 (2013) 211802]
[Campanario, Figy, Plätzer, Rauch, Schichtel, Sjödahl – PRD 98 (2018) 033]

Comprehensive study of QCD effects in VBF & VBS:

For NLO simulations perturbative and non-perturbative variations comparable.

[Rauch, Plätzer – EPJ C77 (2017) 293]
[Rauch et al. For VBSCAN study – EPJ C78 (2018) 671]
[Jäger, Karlberg, Plätzer, Scheller, Zaro — EPJ C80 (2020) 756 for HXSWG]




[Bittrich, Kirchgaesser, Papaefstathiou, Plätzer, Todt — in preparation]

# Phenomenology at the LHC and beyond



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Full NLO
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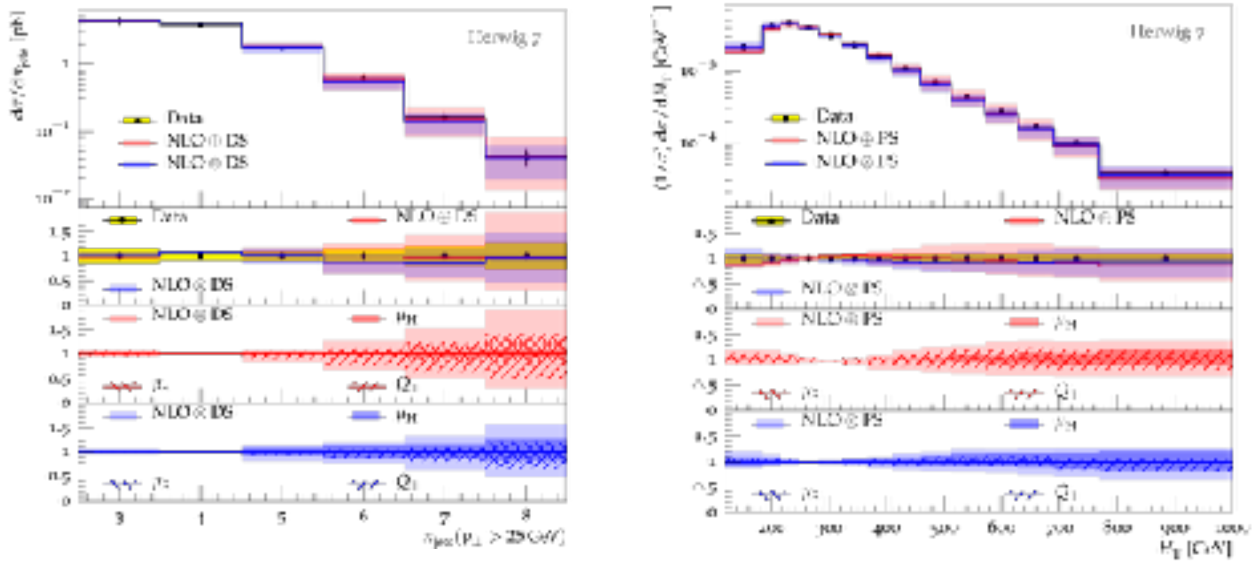
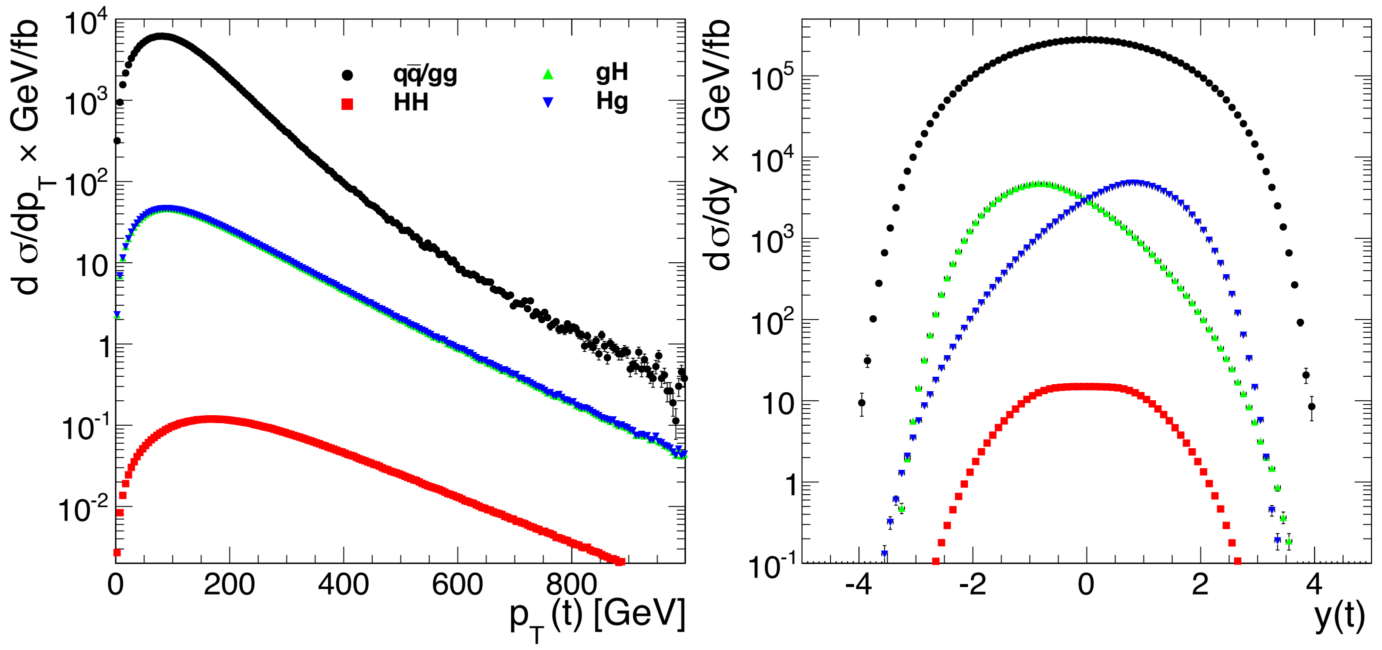
[Rauch, Plätzer
[Rauch et al. F
[Jäger, Karlber

Many more phenomenology applications recently addressed, **always closely linked with development** of the Herwig event generator:

Uncertainty breakdown in top production at NLO and partonshowering off heavy quarks.

[Cormier, Plätzer, Reuschle, Richardson, Webster — EPJ C79 (2019) 915]



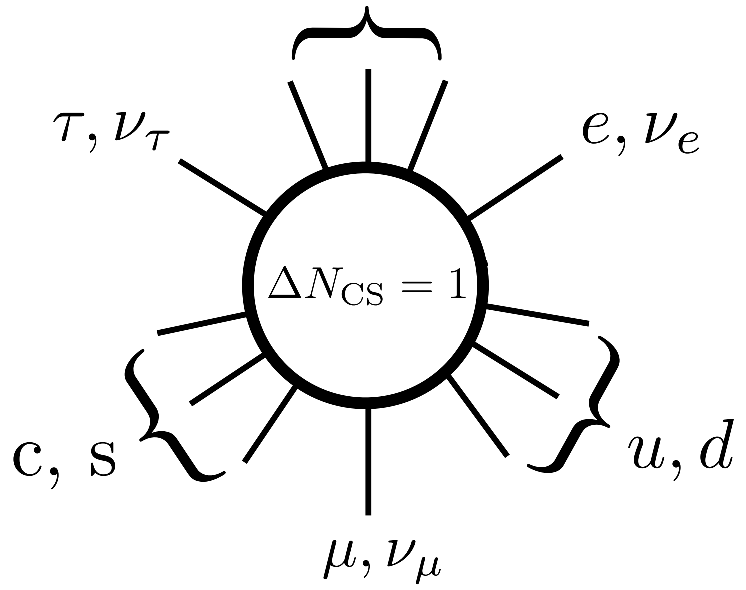




Higgs content in the proton? Phenomenology & experimental constraints.

[Fernbach, Lechner, Maas, Plätzer, Schöfbeck — Phys.Rev.D 101 (2020) 11, 114018]

Sphaleron and instanton induced processes in pp collisions.

[Papaefstathiou, Plätzer, Sakurai — JHEP 1912 (2019) 017]

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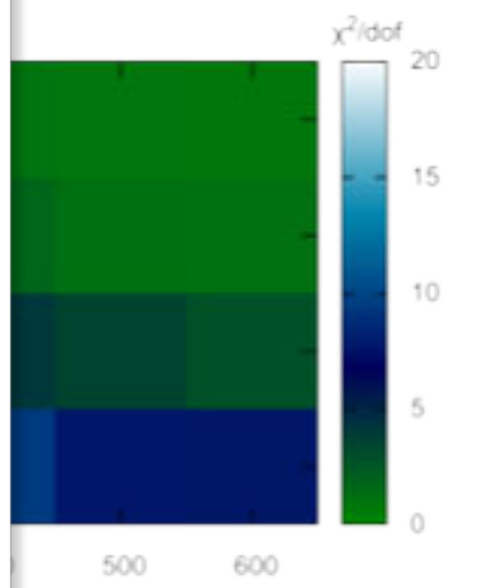

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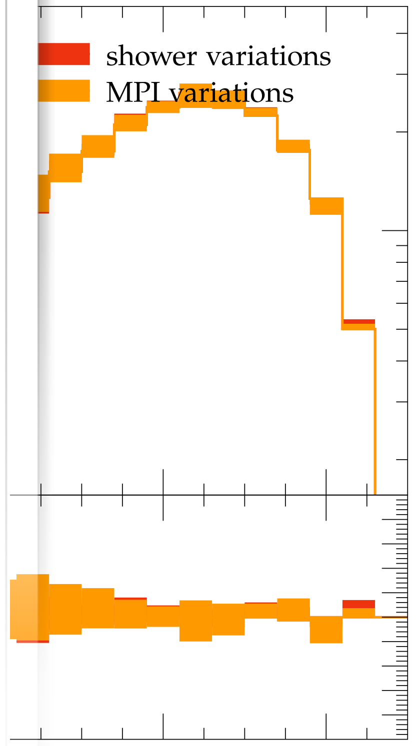
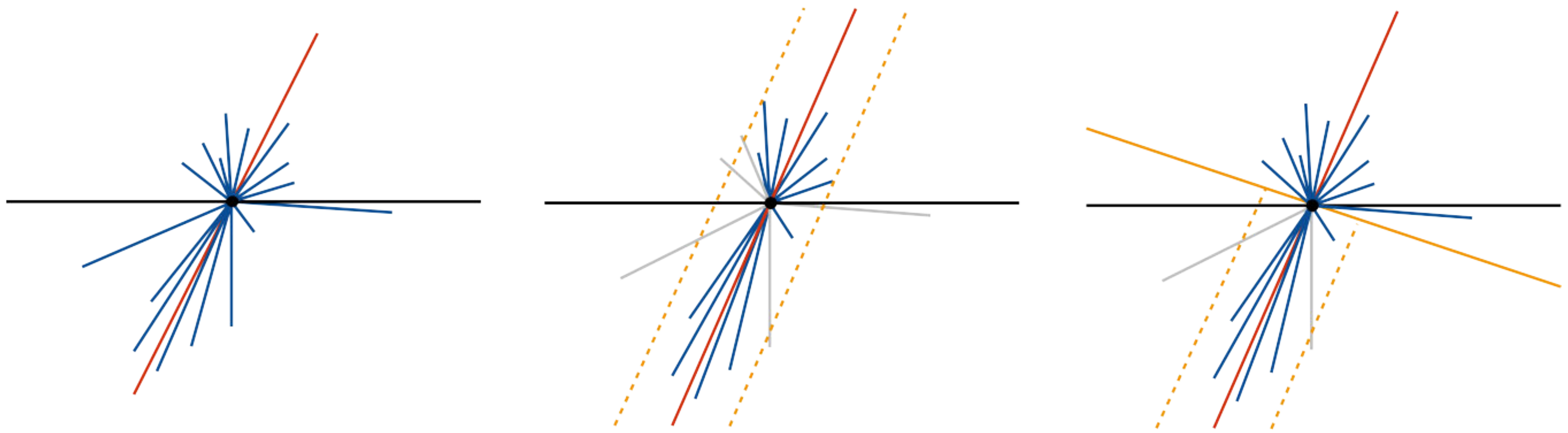



y(3rd jet)

... preparation]

# More precise shower algorithms to fully leverage NNLO



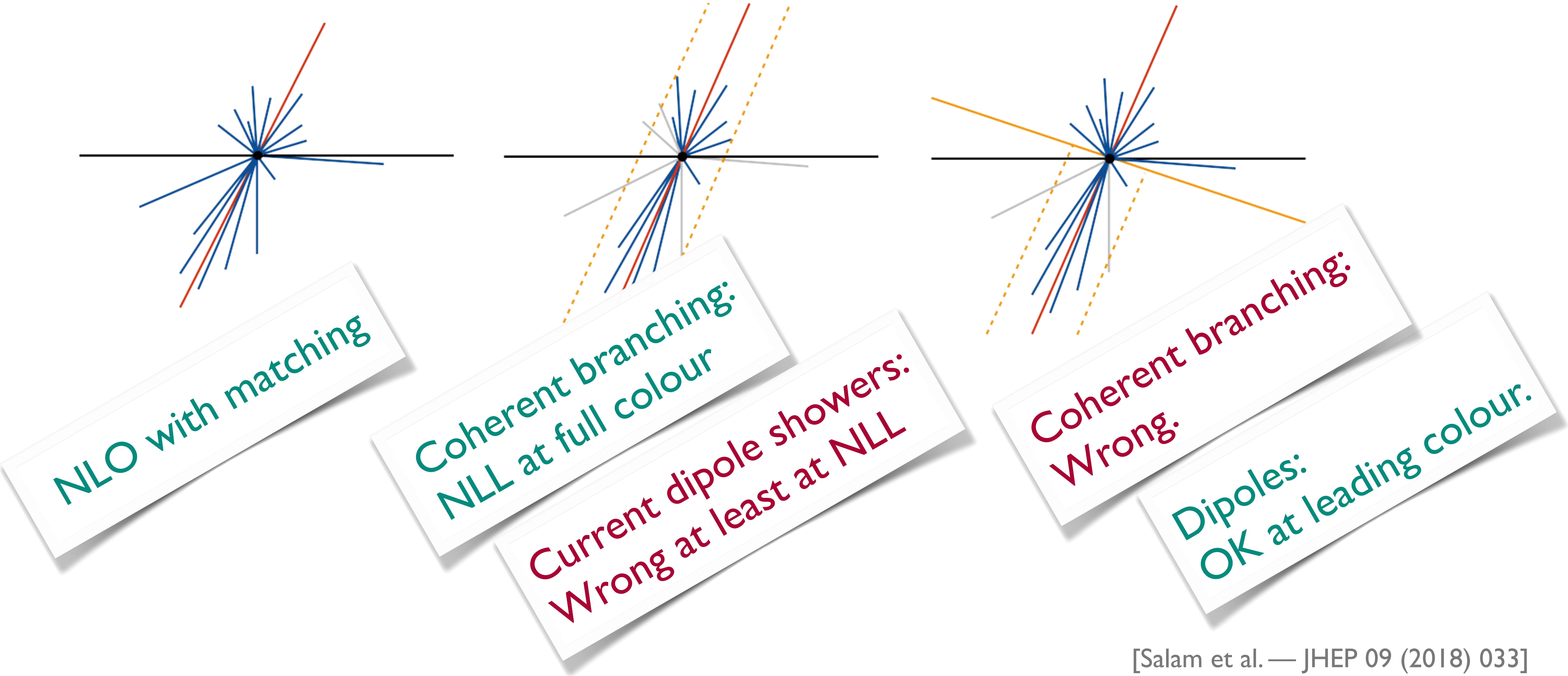


Coherence paradigm fails in general – for any realistic measurement

- Unconstrained systems of non-collinear partons radiate into observed region.
- The full complexity of QCD amplitudes and interference strike back.

1/N effects are comparable to subleading logarithms, and intrinsically 10% effects.

# Before discussing precision … how accurate are we, at all?




[Salam et al. — JHEP 09 (2018) 033]
solutions also offered in [Forshaw, Holguin, Plätzer – JHEP 09 (2020) 014]

# Complexity Factorized?

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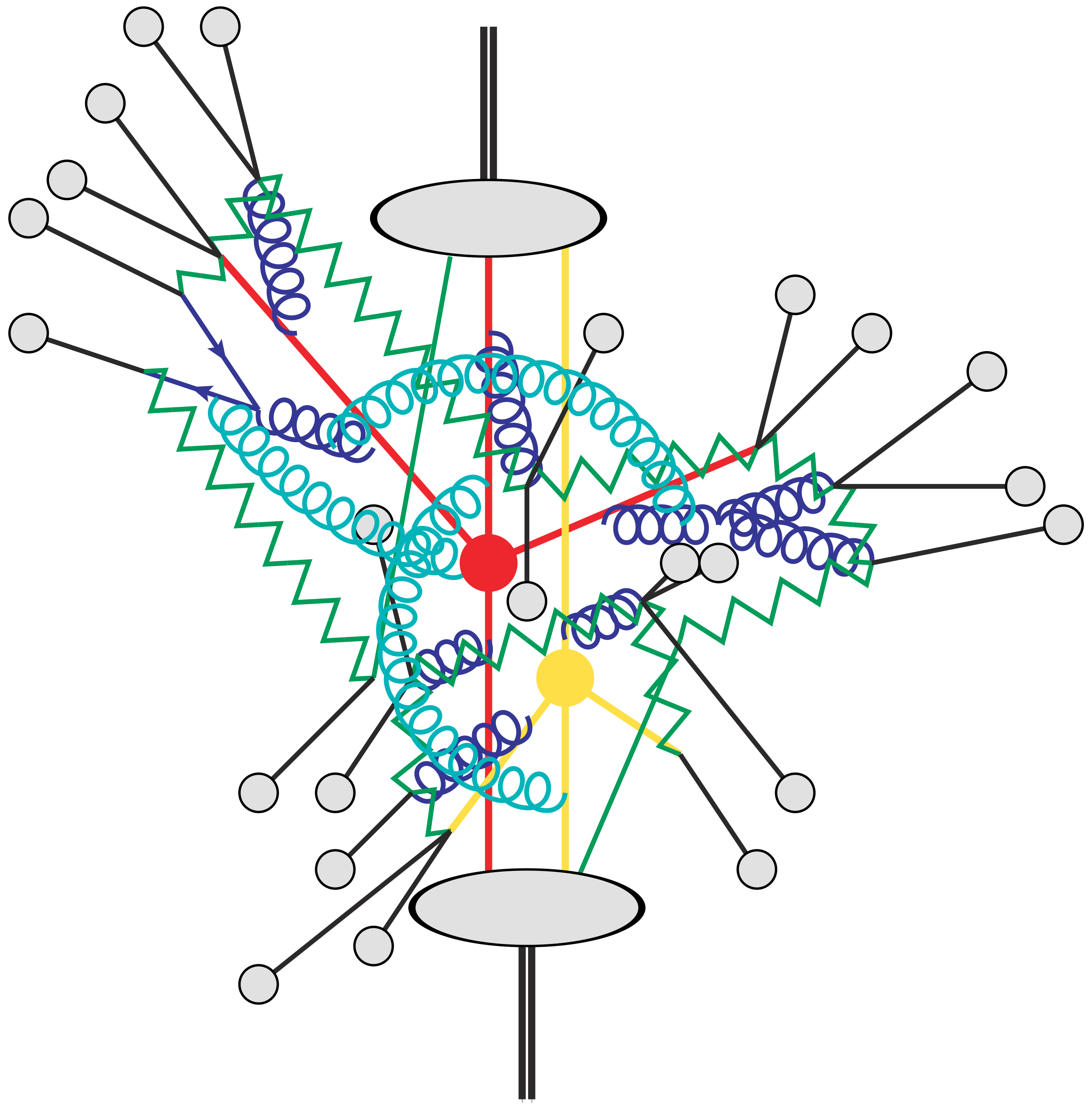

### Parton shower algorithms

Lack a systematic expansion, obstruct fully differential NNLO for the hard process, open questions regarding mass effects and unstable particles, electroweak contributions …

### Hadronization models

Lack constraints from perturbative evolution: Hiding perturbative corrections? Genuine uncertainties/constraints?

### Rethink foundations of parton showers:

Seek a systematic picture including virtual corrections beyond unitarity, and quantum mechanical interference.

$$\mathrm{d}\sigma \sim \mathrm{Tr}[\mathbf{PS}(Q \to \mu)\mathrm{d}\mathbf{H}(Q)\mathbf{PS}^\dagger(Q \to \mu)\mathbf{Had}(\mu \to \Lambda)]$$

# Parton Branching at Amplitude Level

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[Angeles, De Angelis, Forshaw, Plätzer, Seymour – JHEP 05 (2018) 044]
[Forshaw, Holguin, Plätzer – JHEP 1908 (2019) 145]
[see also Nagy & Soper]

$$\sigma = \sum_n \int \mathrm{Tr}\left[\mathbf{A}_n(\mu)\right] u(p_1, \ldots, p_n)\, \mathrm{d}\phi_n$$

density operator — observable — phase space integration

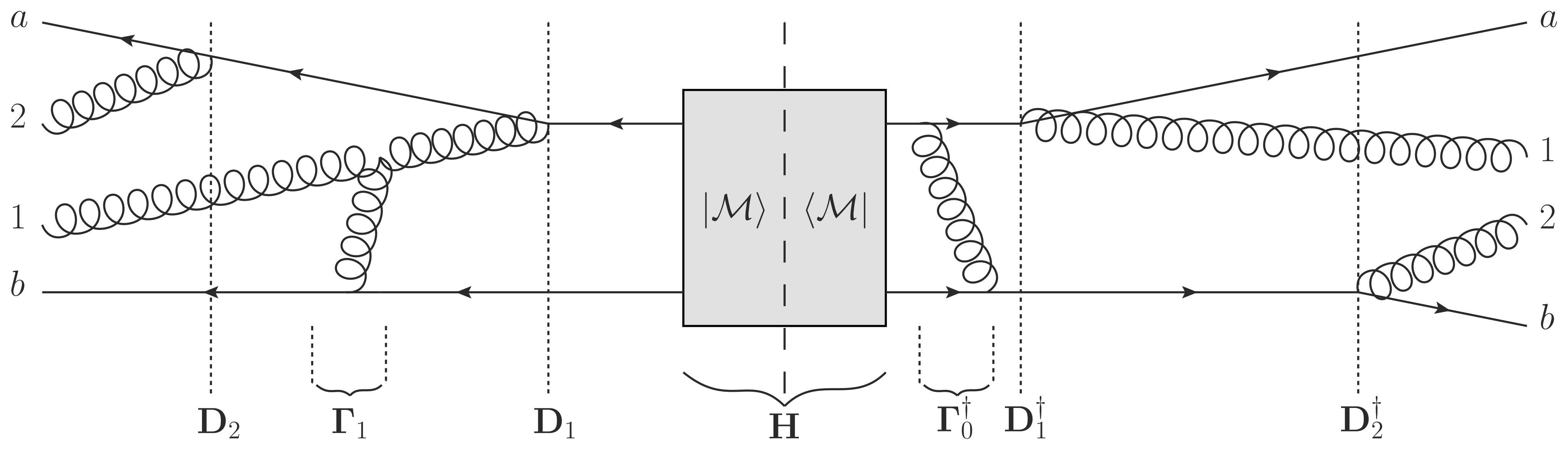
Density operator is fundamental object, not the amplitude, nor the cross section.

Virtual corrections and colour mixing in all orders perturbation theory. $|\mathcal{M}_n(\mu)\rangle = \mathbf{Z}^{-1}(\mu, \epsilon)|\tilde{\mathcal{M}}_n(\epsilon)\rangle$

Recursive definition of evolution at amplitude & conjugate amplitude

$$\mathbf{A}_n(E) = \mathbf{V}(E, E_n)\mathbf{D}_n\mathbf{A}_{n-1}(E_n)\mathbf{D}_n^\dagger\mathbf{V}^\dagger(E, E_n)\theta(E - E_n)$$

Solution to a **renormalisation group equation** which allows to control precision through order of evolution and accuracy through explicit infrared subtractions.



# Parton Branching at Amplitude Level

[Angeles, De Angelis, Forshaw, Plätzer, Seymour – JHEP 05 (2018) 044]
[Forshaw, Holguin, Plätzer – JHEP 1908 (2019) 145]
[see also Nagy & Soper]

$$\sigma = \sum_n \int \mathrm{Tr}\left[\mathbf{A}_n(\mu)\right]\, u(p_1, ..., p_n)\, \mathrm{d}\phi_n$$

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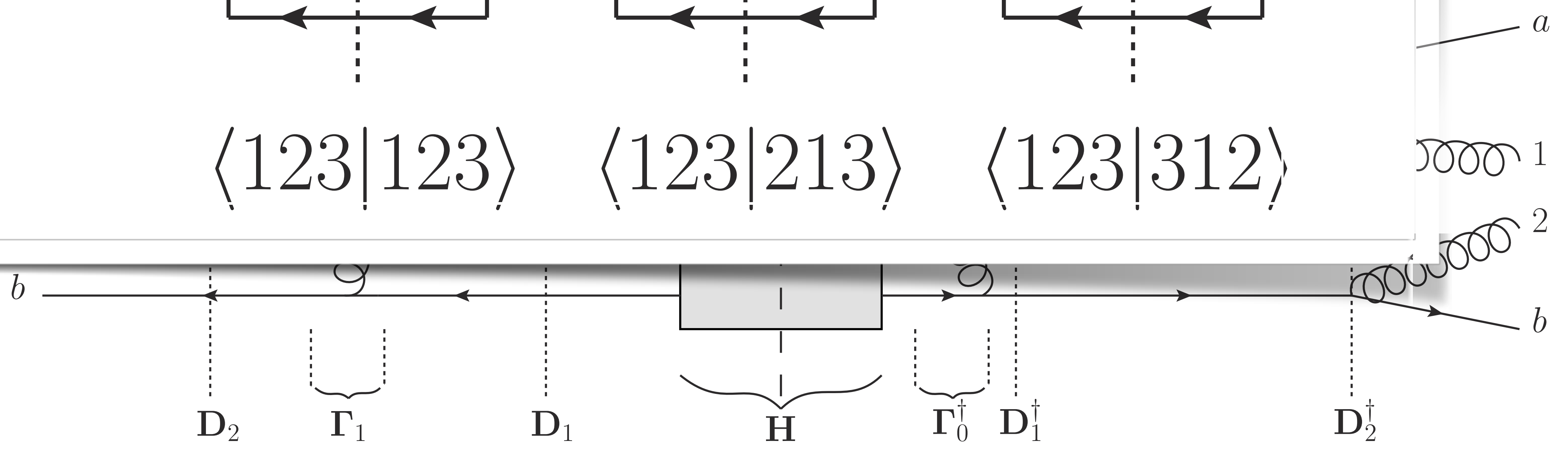
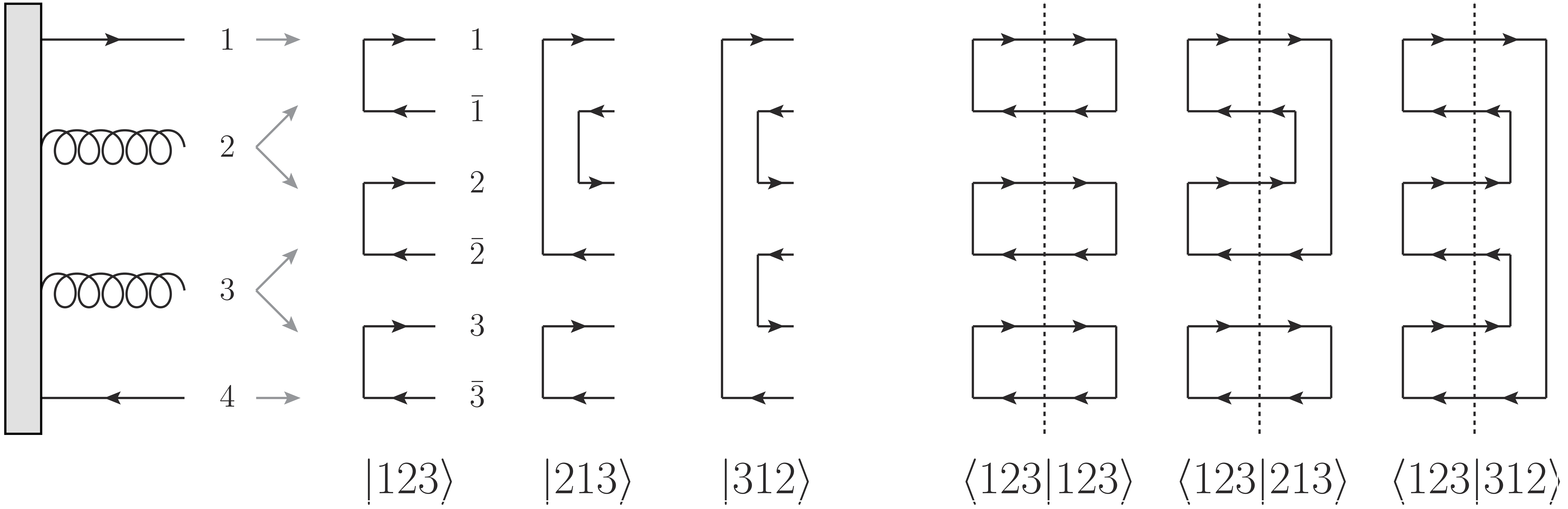
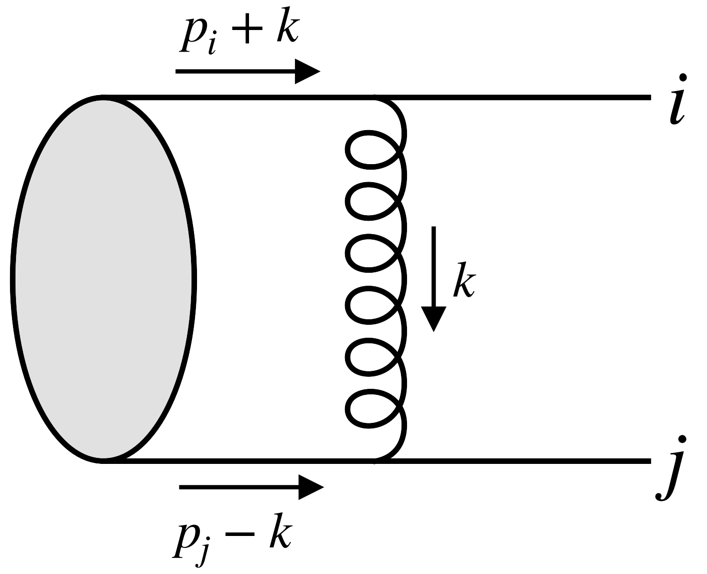



Colour space is about tracking flow of colour charge:



# Novel Algorithmic Frameworks

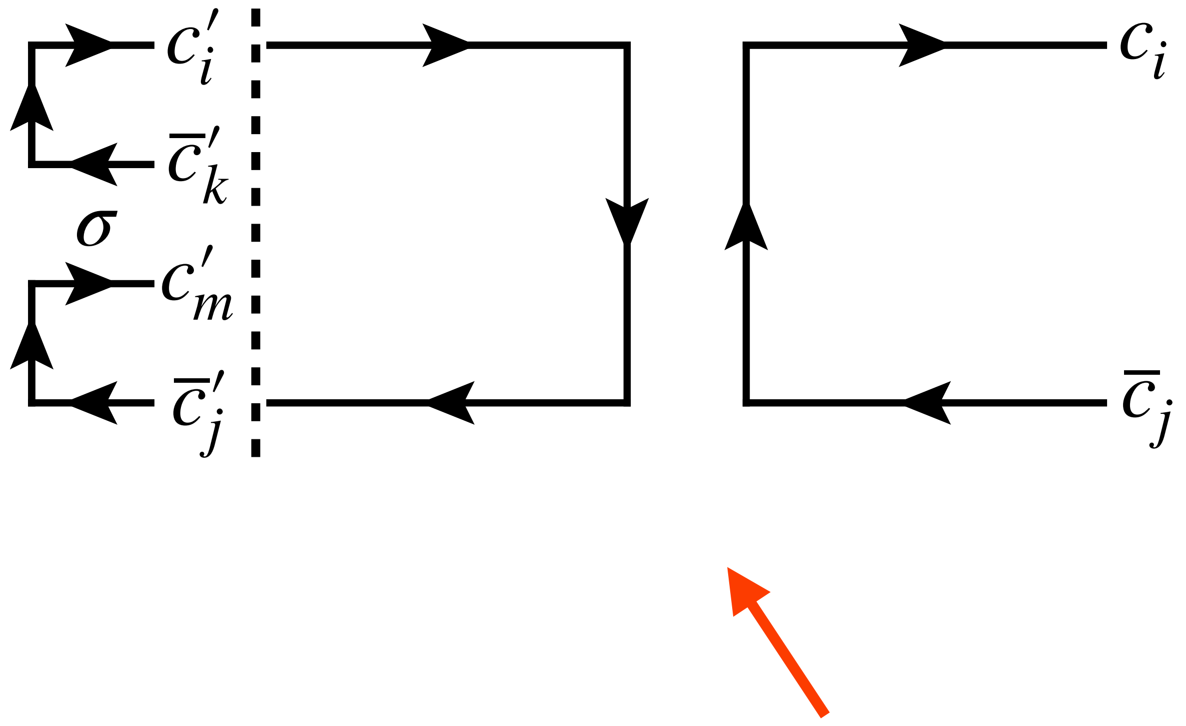
Colour structure of one-loop exchanges:




[Plätzer – EPJ C 74 (2014) 2907]

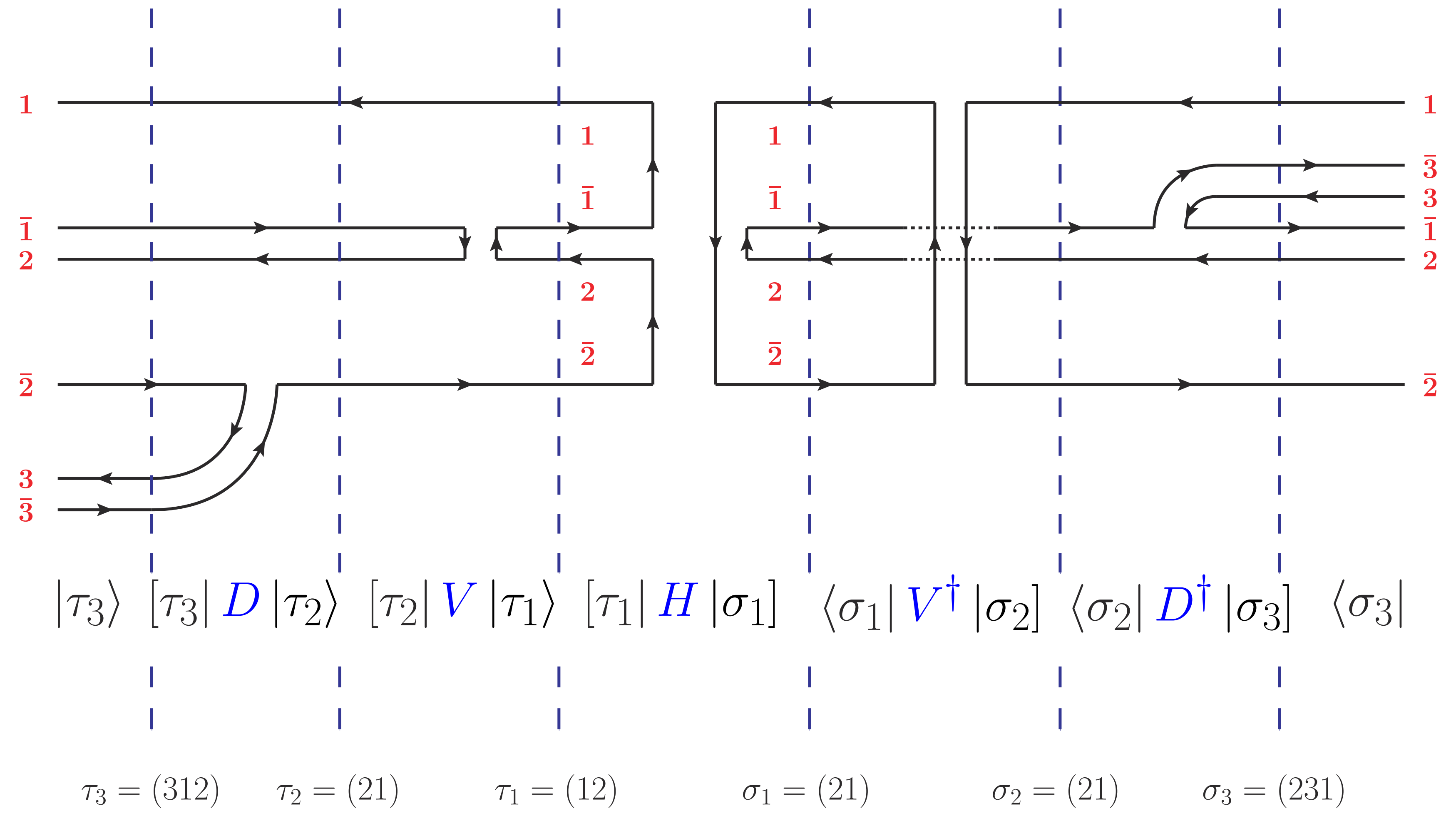
$$[\tau|\mathbf{\Gamma}|\sigma\rangle = N\delta_{\tau\sigma}\Gamma_\sigma + \Sigma_{\tau\sigma} + \frac{1}{N}\delta_{\tau\sigma}\rho$$

Systematically expand around large-N limit summing towers of terms enhanced by $\alpha_S N$




dipole flips at next-to-leading colour

[De Angelis, Forshaw, Plätzer — arXiv:2007.09648]




amplitude conjugate amplitude

Avoid complexity which grows with colour space dimensionality:

- Monte Carlo over colour flows,
- events at intermediate steps carry complex weights.

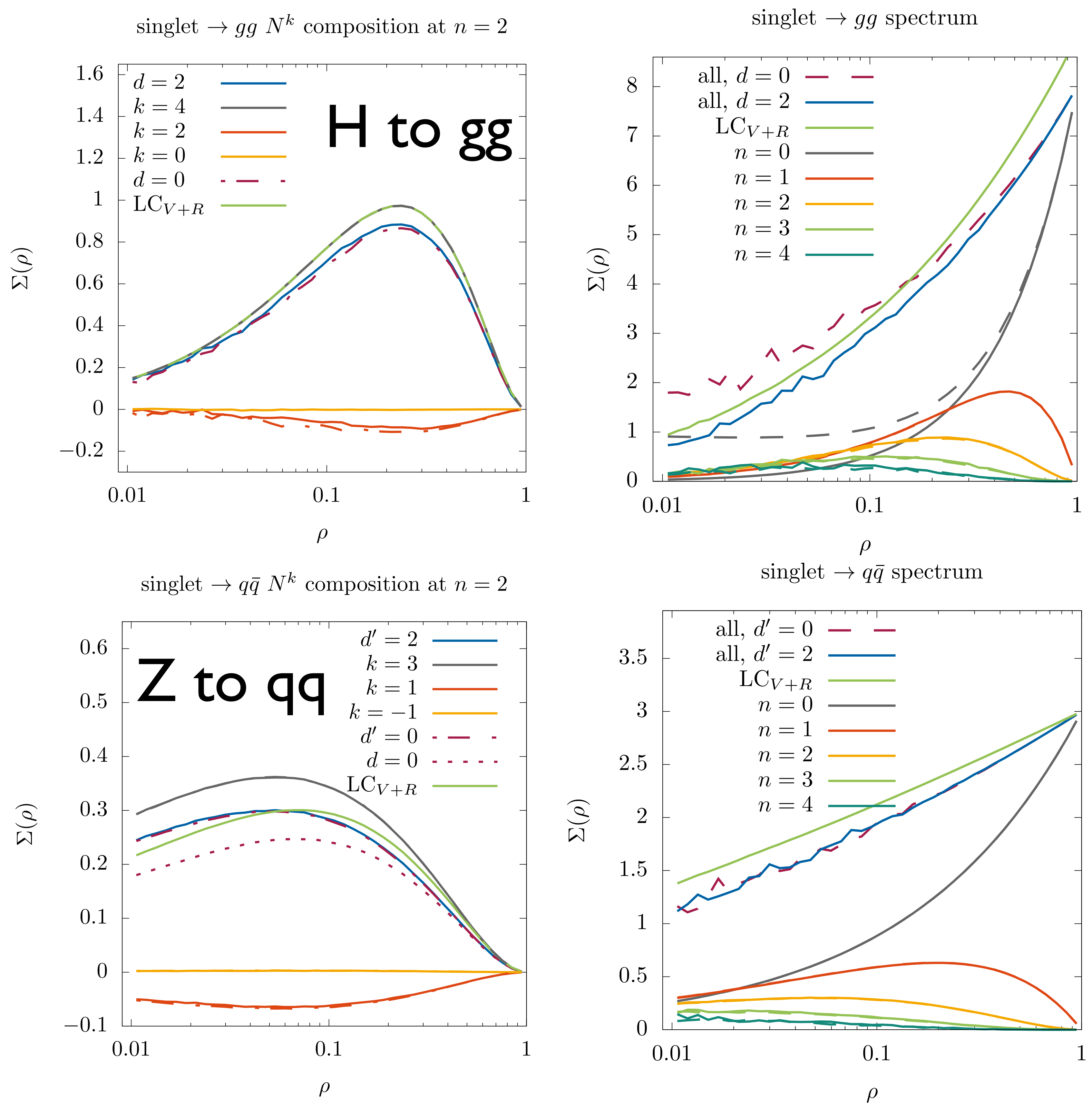
# Novel Algorithmic Frameworks

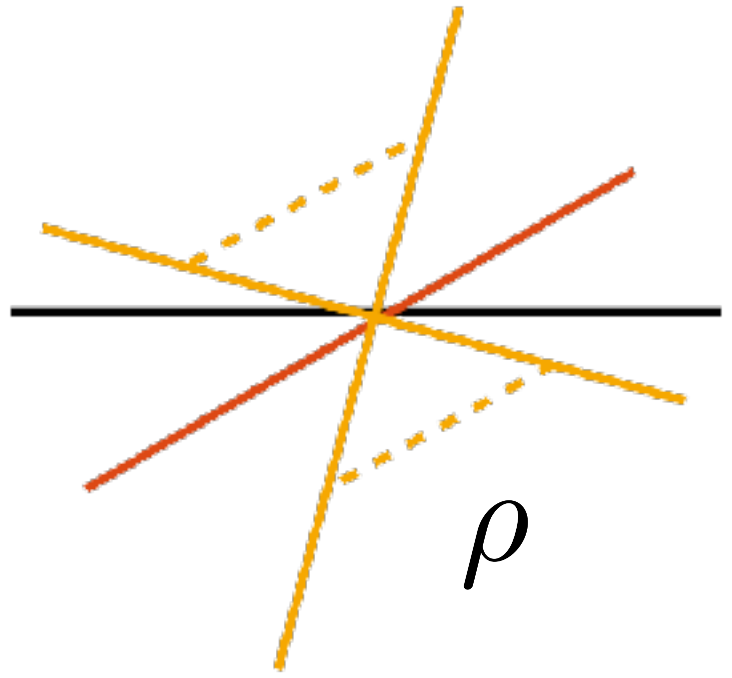
[De Angelis, Forshaw, Plätzer — arXiv:2007.09648]

CVolver library implements numerical evolution in colour space.

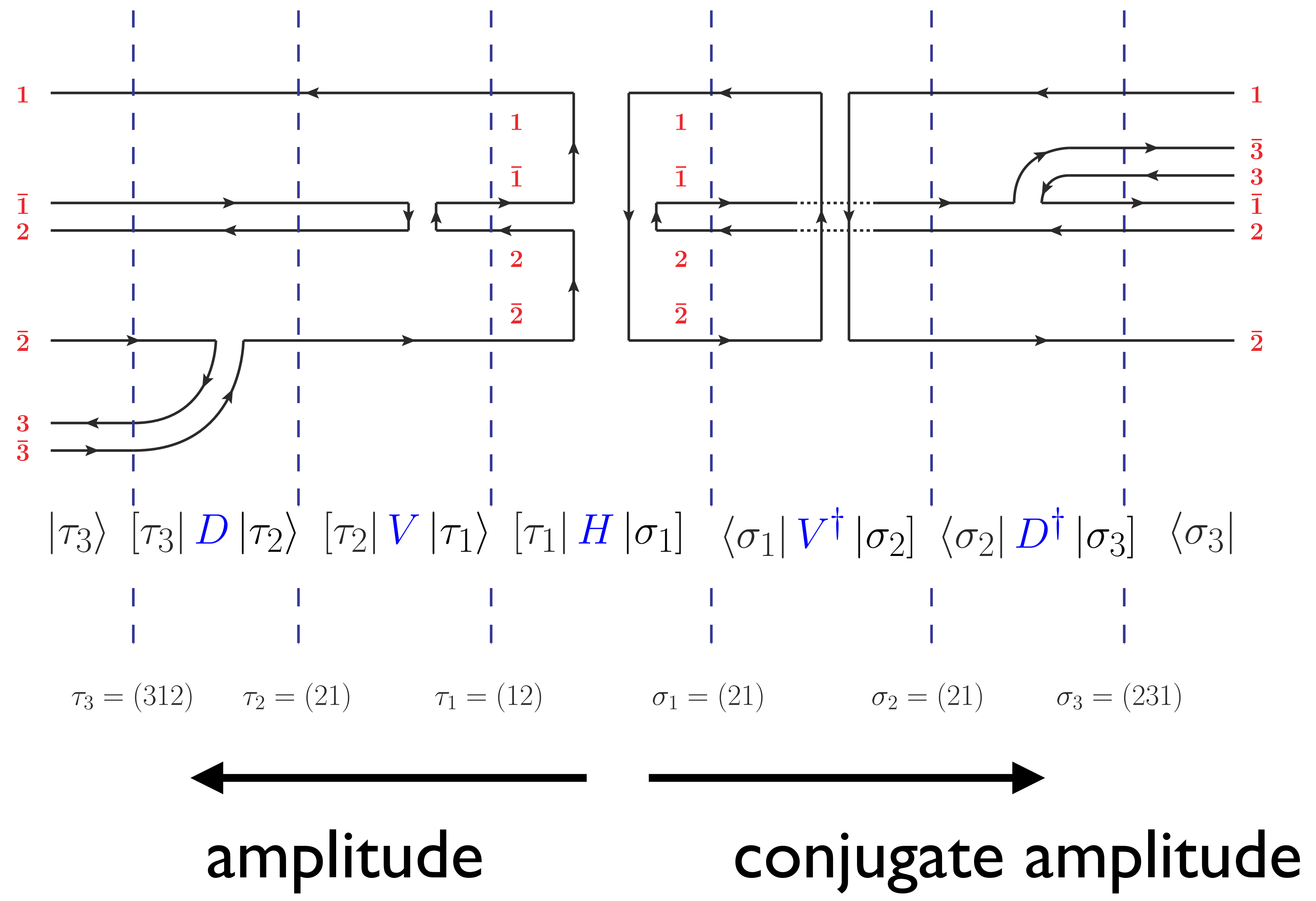
origins in [Plätzer – EPJ C 74 (2014) 2907]

Resummation of non-global logarithms at full colour:




$$\Sigma(\rho) = \sum_n \int \mathrm{d}\sigma(\{p_i\}) \prod_i \theta_{\mathrm{in}}(\rho - E_i)$$




Avoid complexity which grows with colour space dimensionality:

- Monte Carlo over colour flows,
- events at intermediate steps carry complex weights.

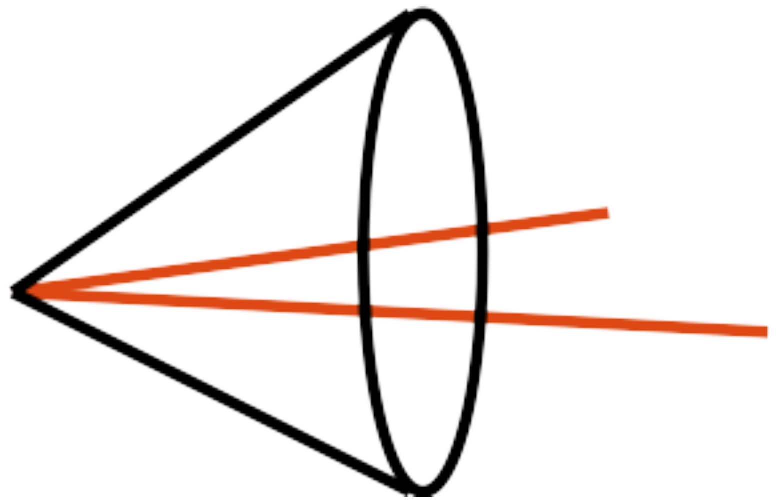
# Tackling Complexity

Computer algebra & code generation

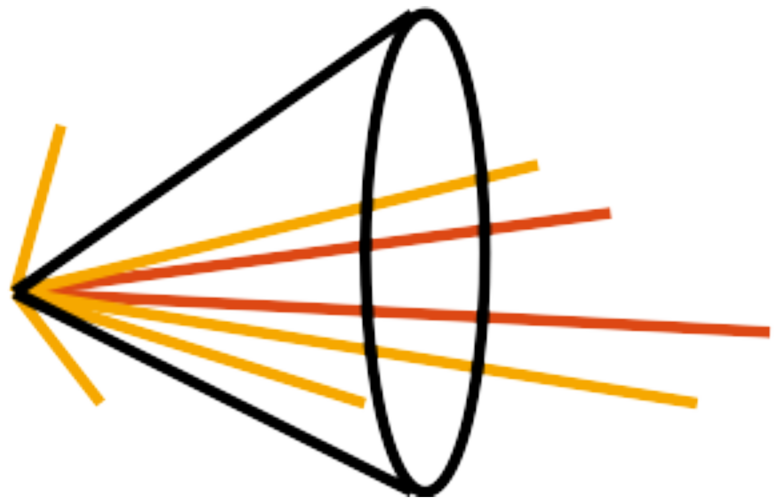
Design & implementation of physics analyses

Combinatorial/diagramatic algorithms

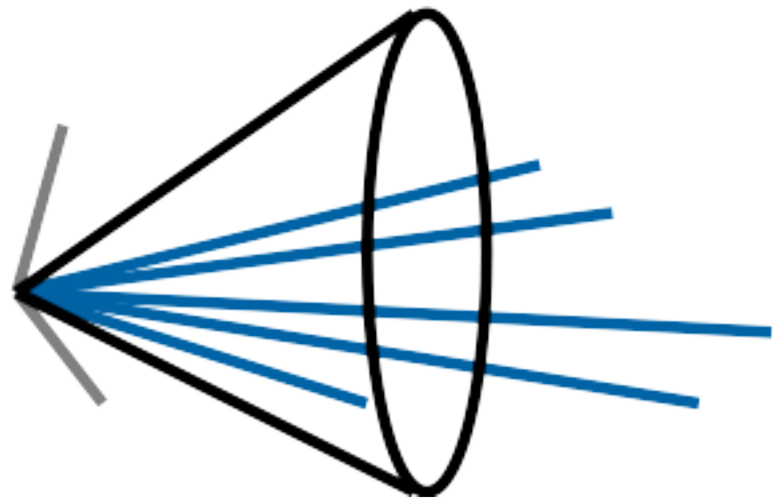
**Jet production**



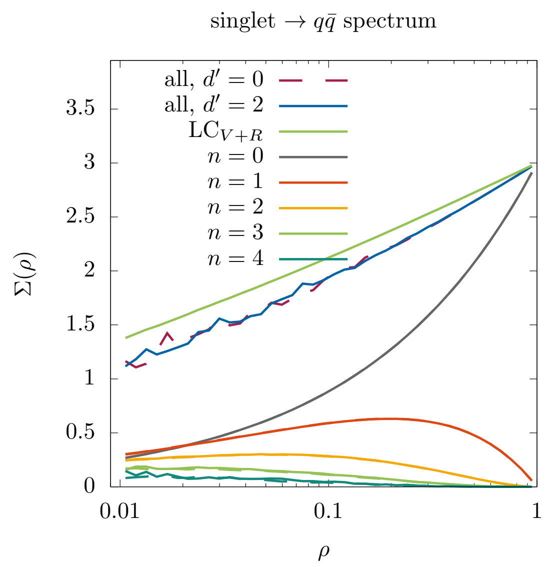
**Jet evolution**



**Hadronization, soft QCD**



**Phenomenology**




Monte Carlo integration

MC simulation & adaptive sampling

Cluster/HPC planning & operation

Reliable histogramming & statistics

Fitting & parameter scans

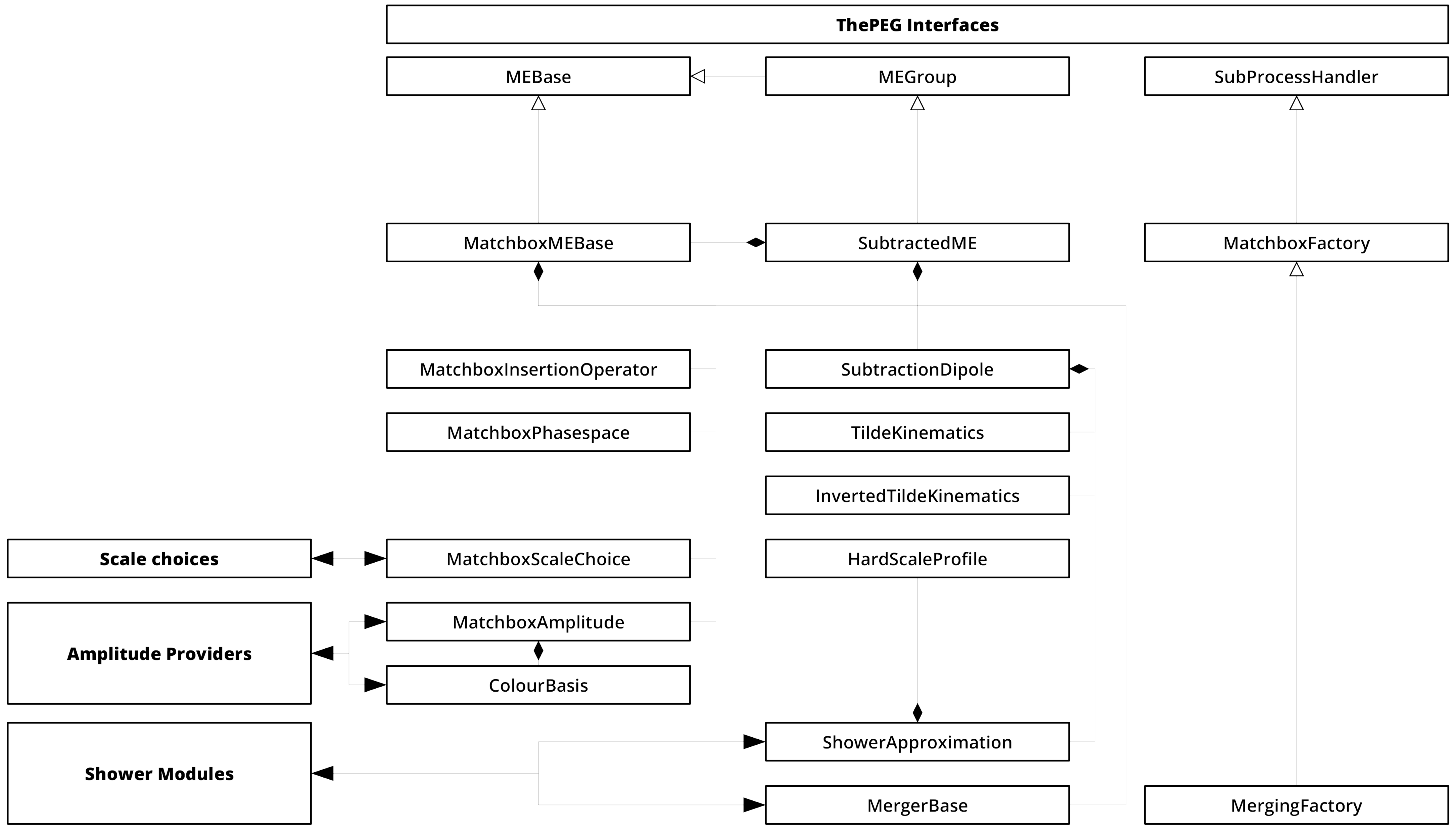
Community-wide tools **always involved:** FastJet, LHAPDF, HepMC, Rivet, loop libraries …

Large span of paradigms/languages: C++, Python, Fortran, Mathematica — loads of automation on distributed/cluster setups.

# Matchbox, DipoleShower & Herwig 7


Lead on the design, development and maintenance of key modules of Herwig 7:

- DipoleShower: workhorse for modern event generator improvements and alternative evolution.
- Matchbox: highly versatile framework for NLO calculations and matching/merging.
- Reweighting algorithms, hadronization improvements, overall framework structure




Includes driving forward and using 'Les Houches accords' for external libraries such as OpenLoops, and in-house low level interfaces to e.g. MadGraph.

Object-oriented design **follows structure of an actual NLO(+PS) calculation** — flexible change of subtraction and matching.

Large C++ project, up to five people involved in Matchbox, managed using Mercurial.

# Matchbox, DipoleShower & Herwig 7


Lead on the design, development and maintenance of key

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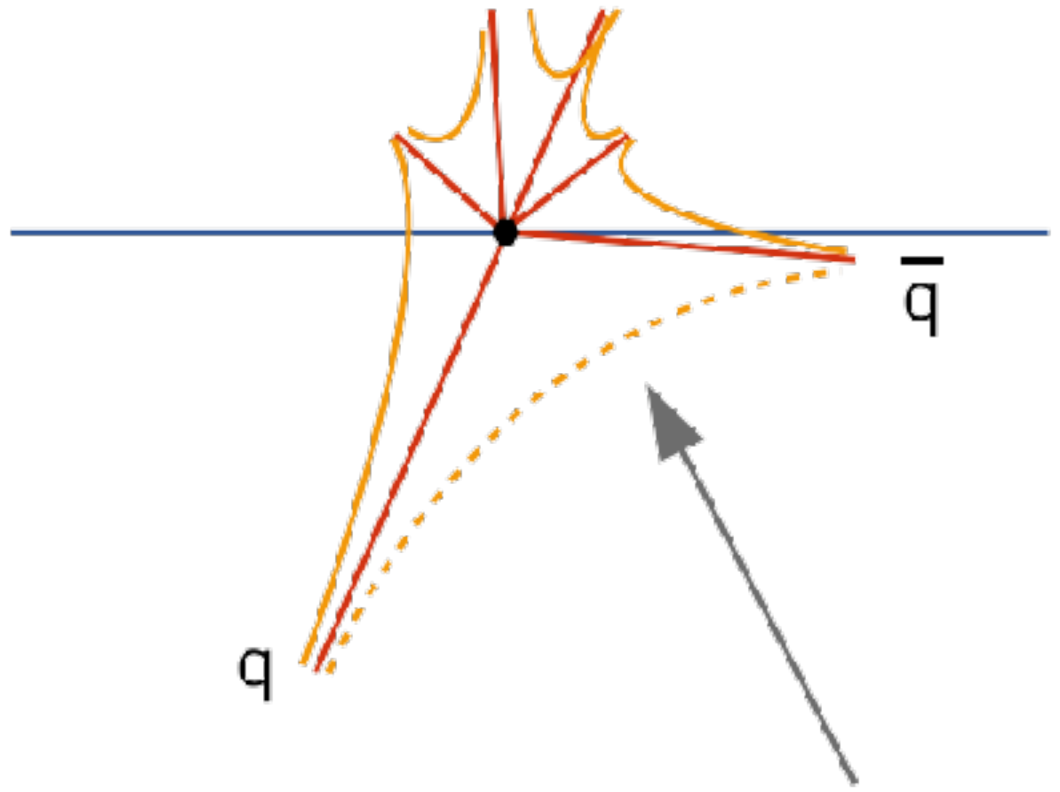
Flexible structure allows e.g. for colour matrix element corrections

$$|\mathcal{M}\rangle = \sum_\sigma \mathcal{M}_\sigma |\sigma\rangle$$

$$d\sigma_{n+1} \sim |\mathcal{M}_{n+1}|^2 = \langle \mathcal{M}_{n+1}|\mathcal{M}_{n+1}\rangle \sim P \, d\sigma_n$$

$$\to \frac{\mathrm{Tr}\left[|\mathcal{M}_n\rangle\langle\mathcal{M}_n|\mathbf{P}\right]}{|\mathcal{M}_n|^2 P} P \, d\sigma_n$$




[Plätzer, Sjödahl – JHEP 1207 (2012) 042]
[Plätzer, Sjödahl, Thoren – JHEP 11 (2018) 009]

Some subleading-N corrections can be restored.

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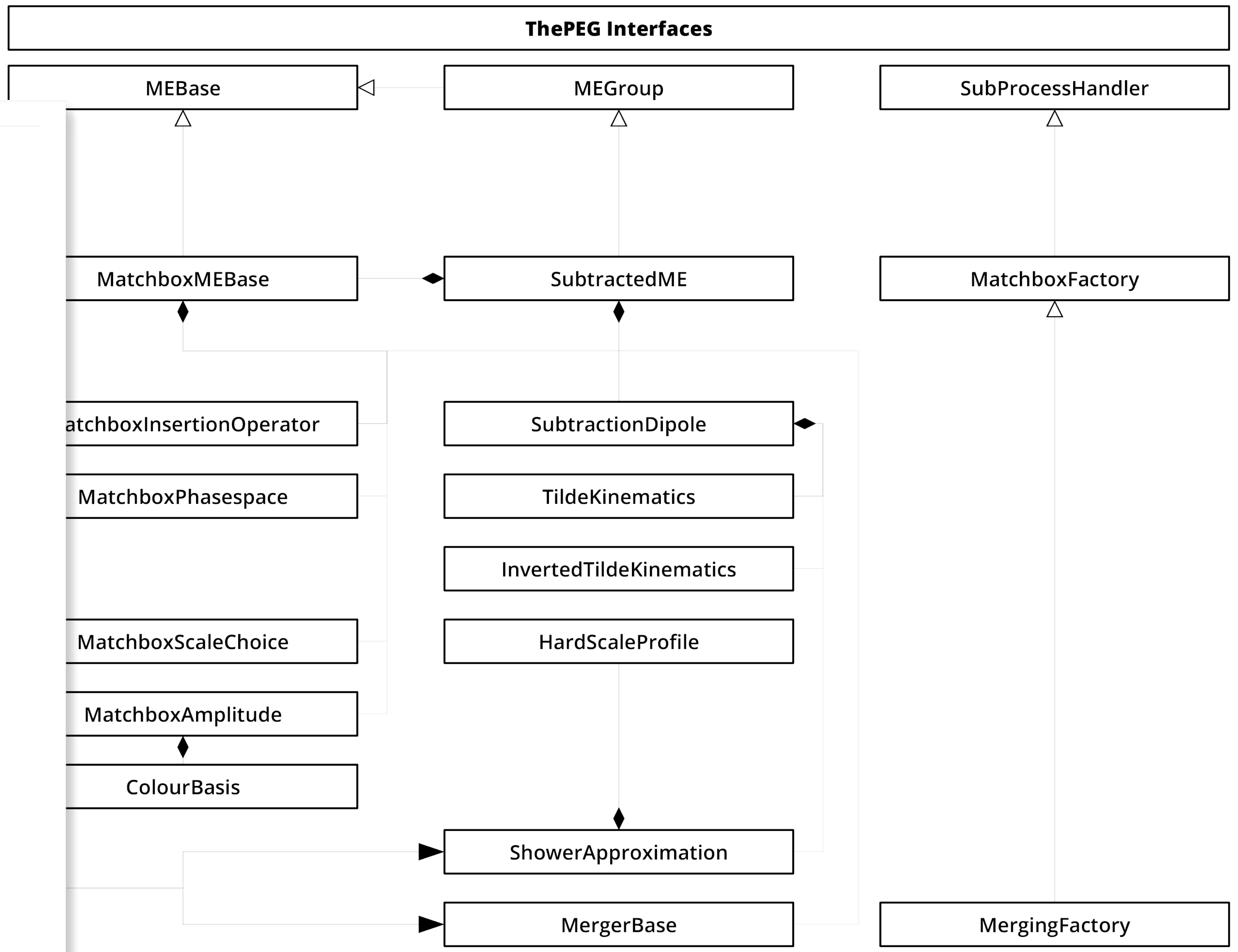



…ted design **follows structure of an (+PS) calculation** — flexible change of subtraction and matching.

Large C++ project, up to five people involved in Matchbox, managed using Mercurial.

# NLO calculations and phenomenology

[Plätzer — mostly unpublished or silently shipped with Herwig]

Amplitudes:

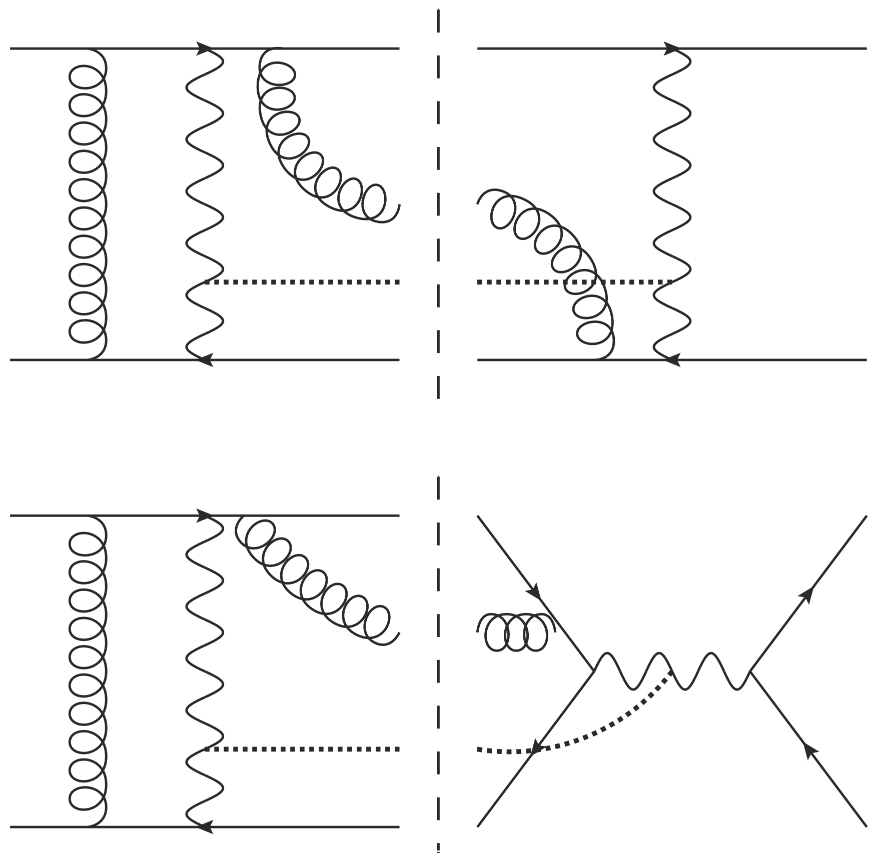
- Code generation in Mathematica synchronised with dedicated C++ spinor helicity library
- Interfaces to 'ME providers' like NJet, OpenLoops …

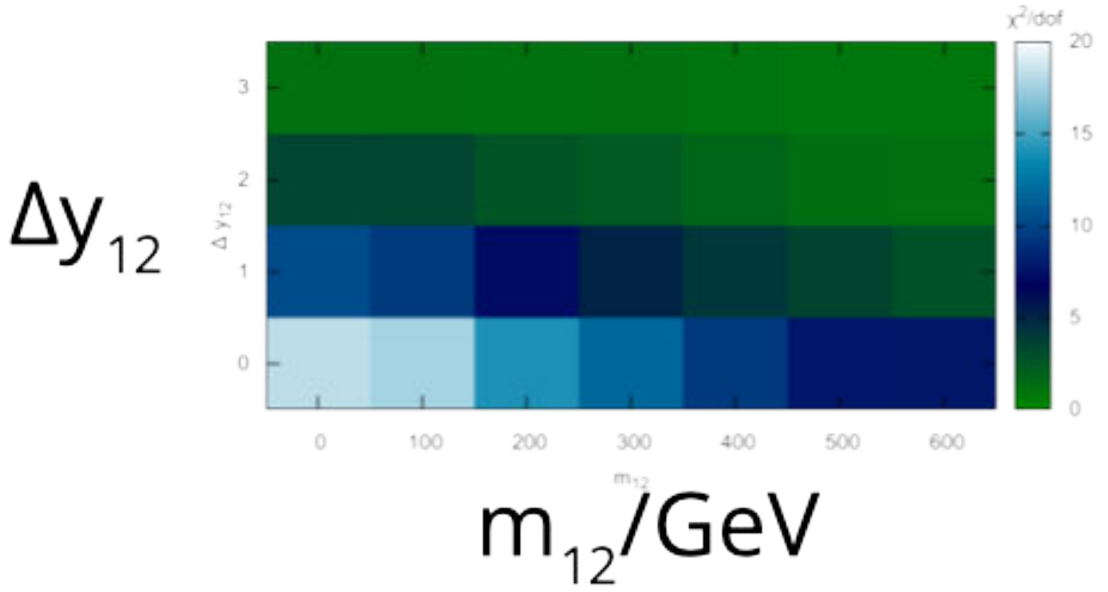
**Numerics within Matchbox:**

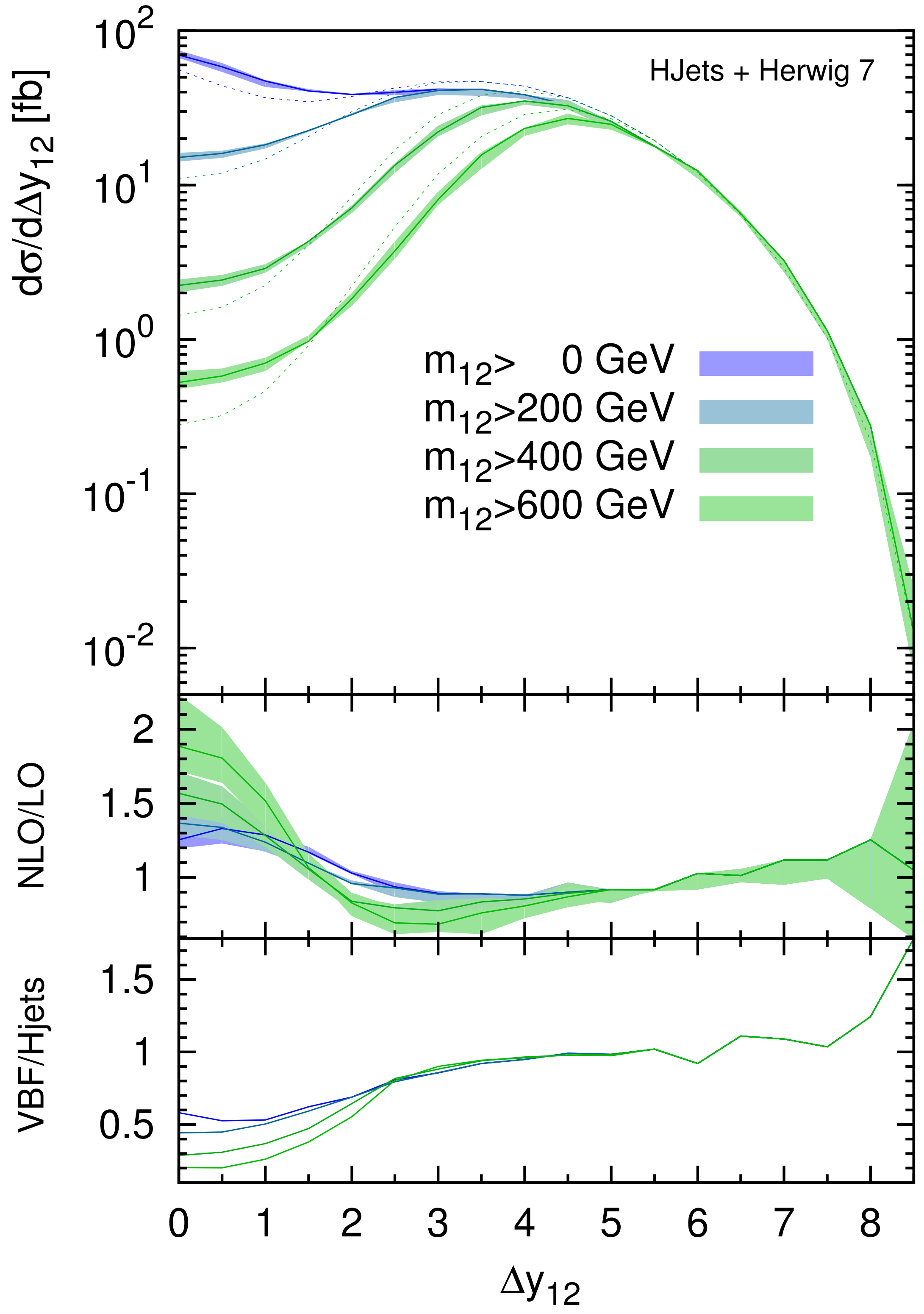
- Automated generation of subtraction terms
- Automated phase space generation
- Combination with virtuals, pole cancellation

Analysis with myStatistics:

- Convergent histogramming
- Data handling, stable combination of parallel runs






[Campanario, Figy, Plätzer, Sjödahl – PRL 111 (2013) 211802]
[Campanario, Figy, Plätzer, Rauch, Schichtel, Sjödahl – PRD 98 (2018) 033]

Combining several libraries, running on Condor cluster @Vienna.

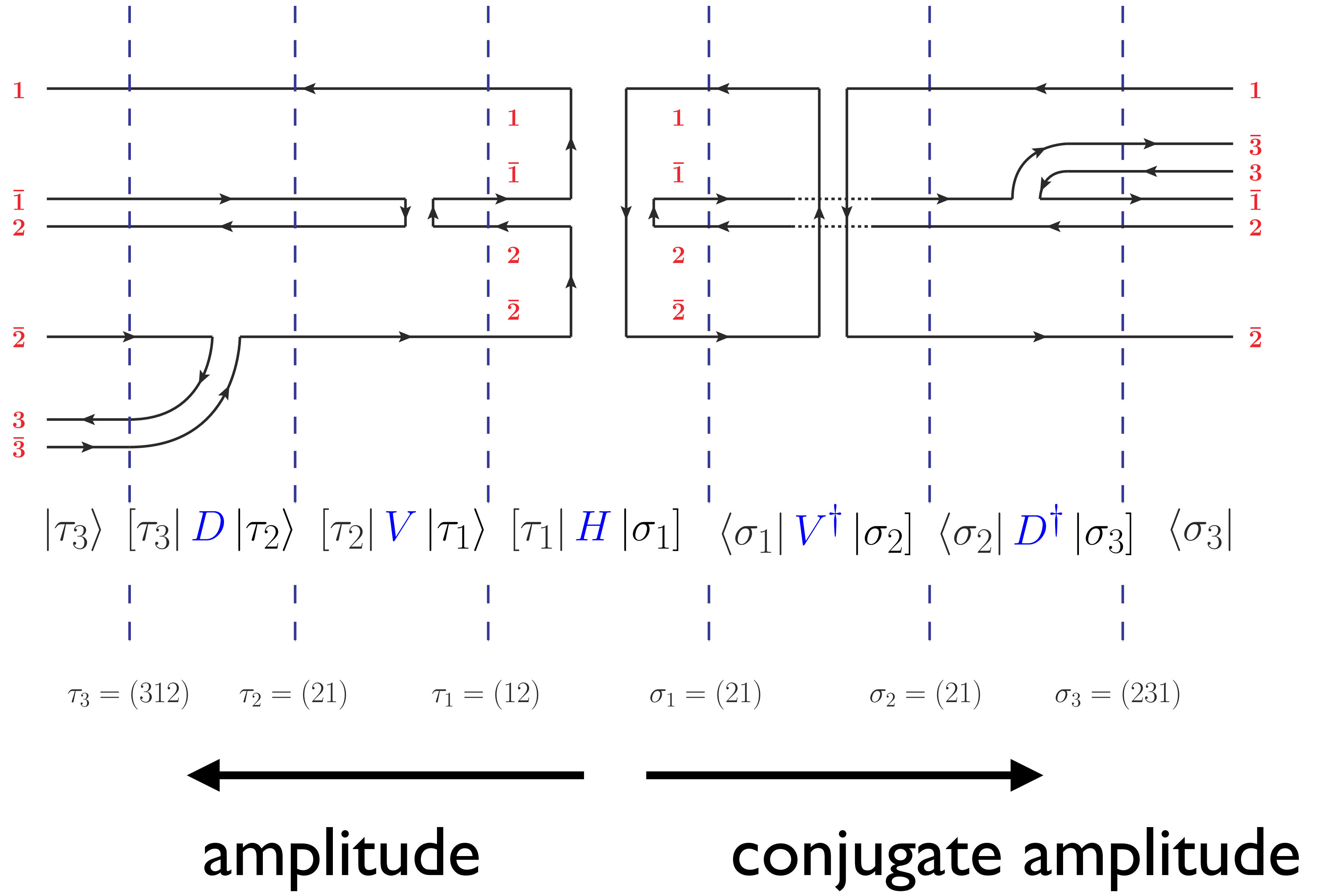
# Under the Hood of CVolver

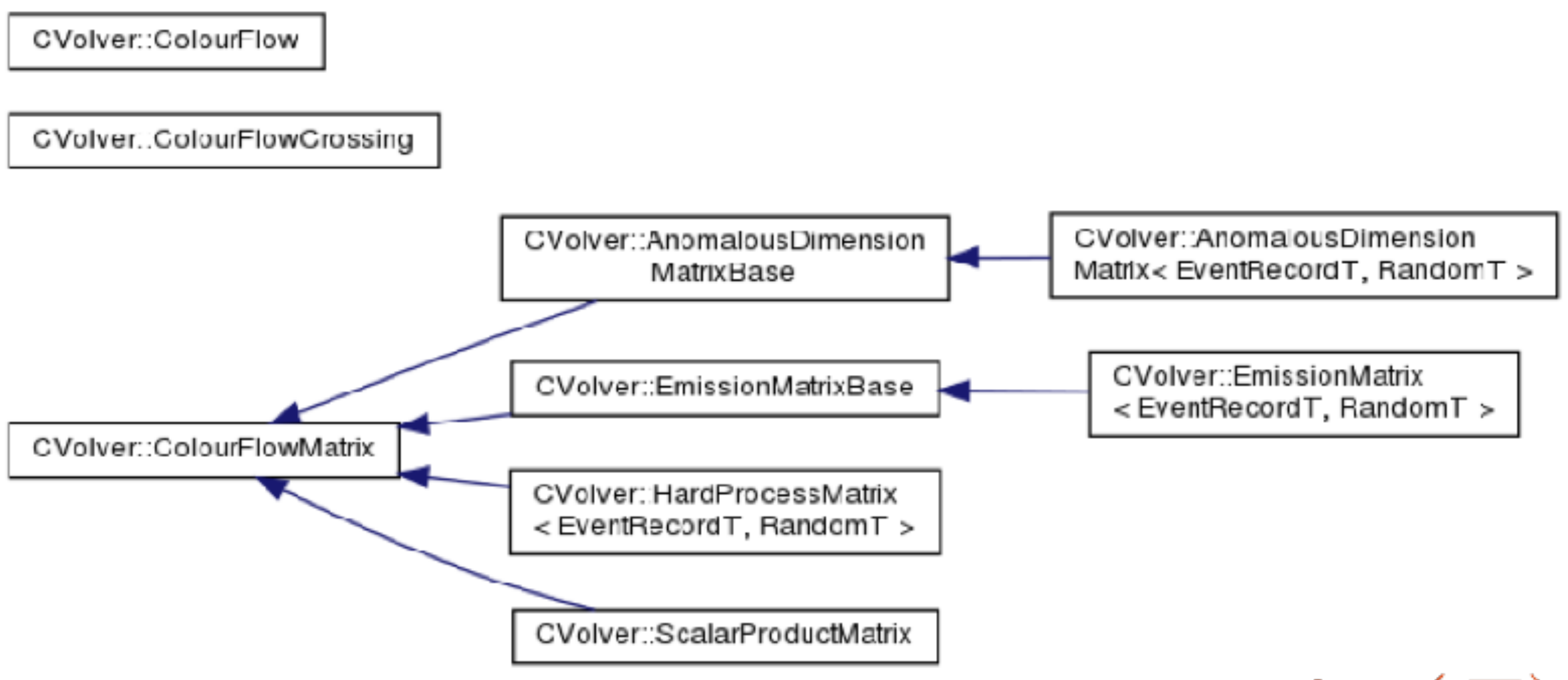
universität wien

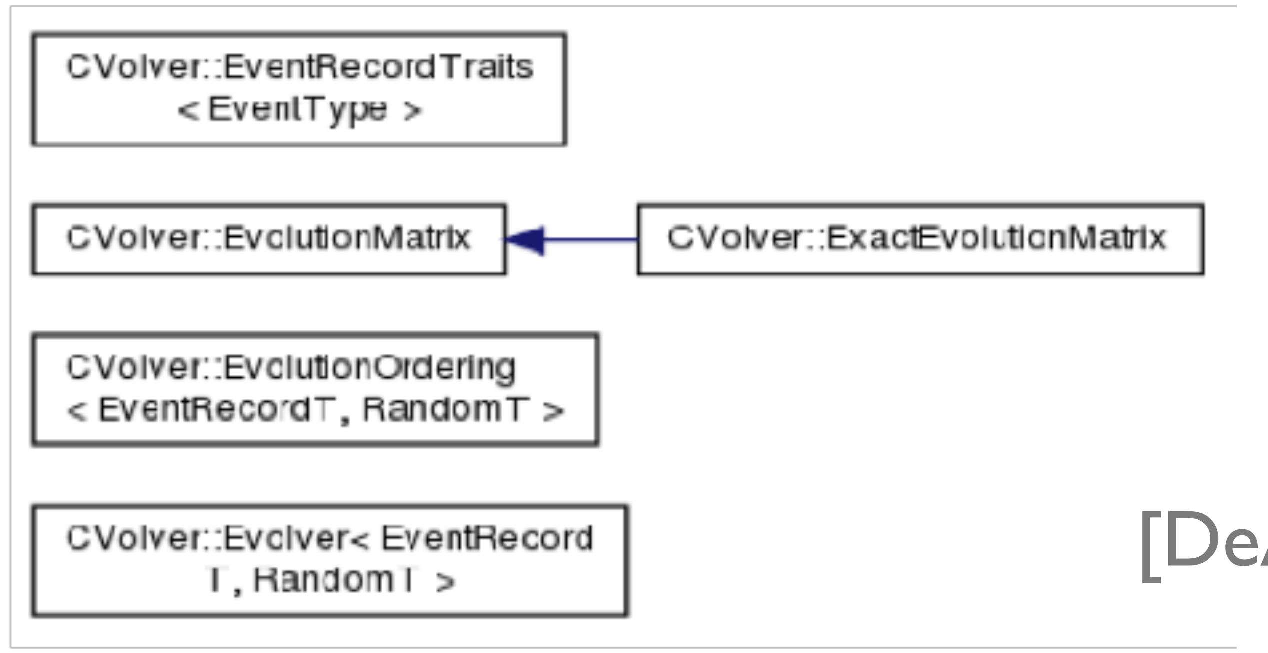
New algorithm demanded modular framework:

Flexible enough to accommodate **exact evolution** for certain classes of observables and to host a **full-fledged parton shower** at amplitude level.

- Modern C++ design paradigms, template meta-programming.
- Avoids monolithic framework to guarantee reusability.




[Plätzer – EPJ C 74 (2014) 2907]
[DeAngelis, Plätzer, Kirchgaesser — in progress]

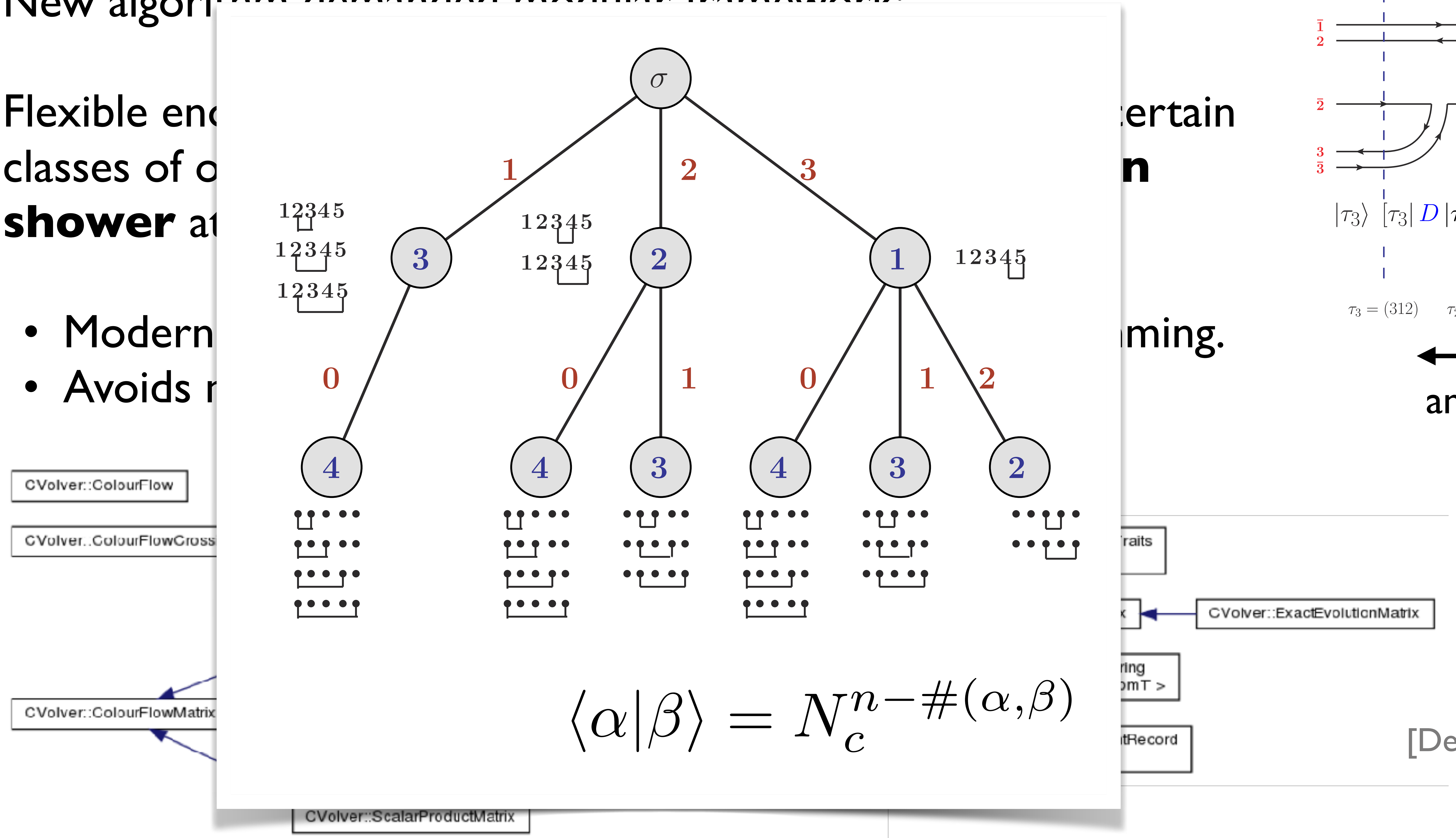
$$\mathbf{A}_n(E) = \mathbf{V}(E, E_n)\mathbf{D}_n\mathbf{A}_{n-1}(E_n)\mathbf{D}_n^\dagger\mathbf{V}^\dagger(E, E_n)\theta(E - E_n)$$

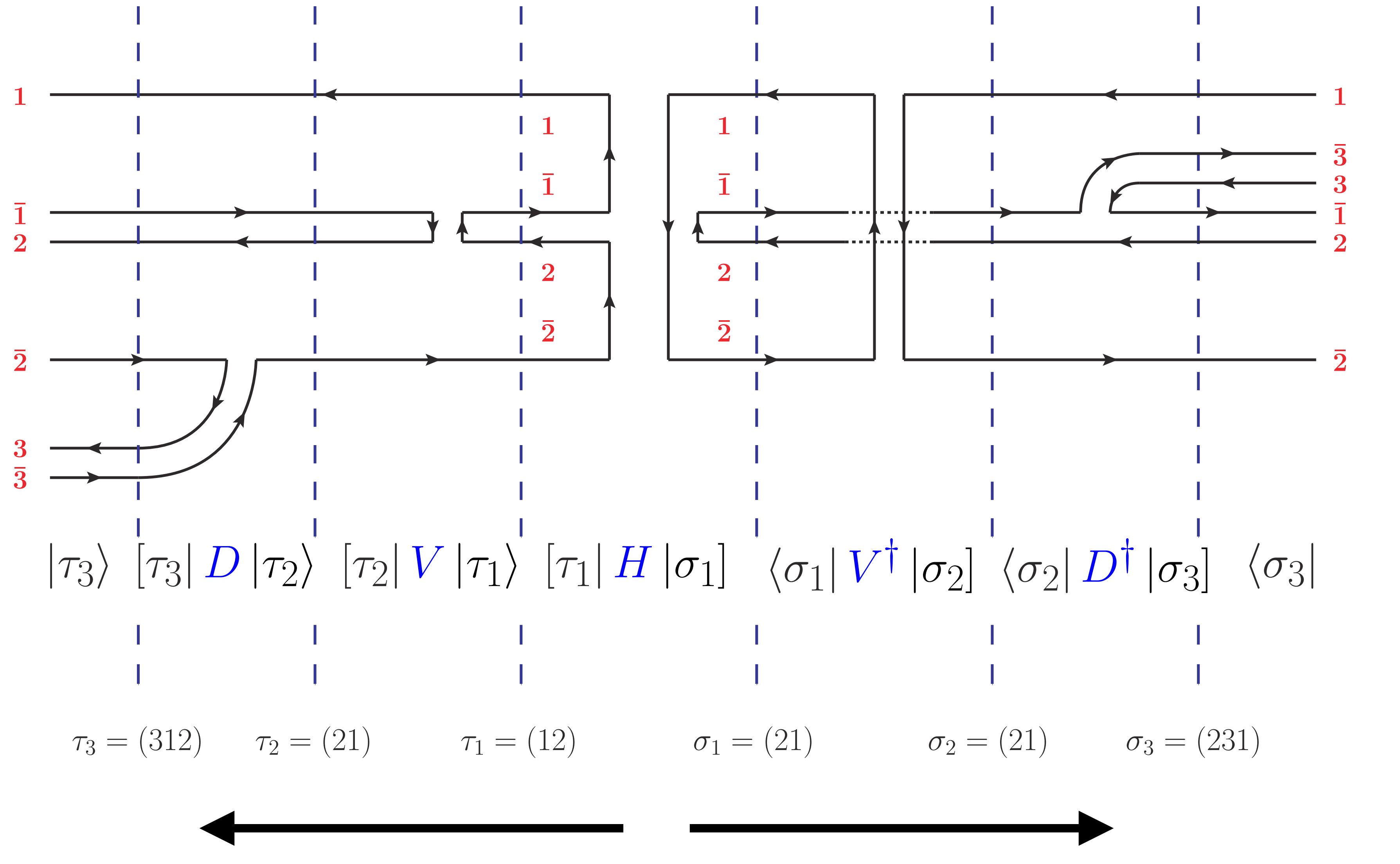
# Under the Hood of CVolver

New algorithm demanded modular framework:

Flexible enc ... certain
classes of o ... n
**shower a** ...

- Modern ... ming.
- Avoids r ...




[Plätzer – EPJ C 74 (2014) 2907]
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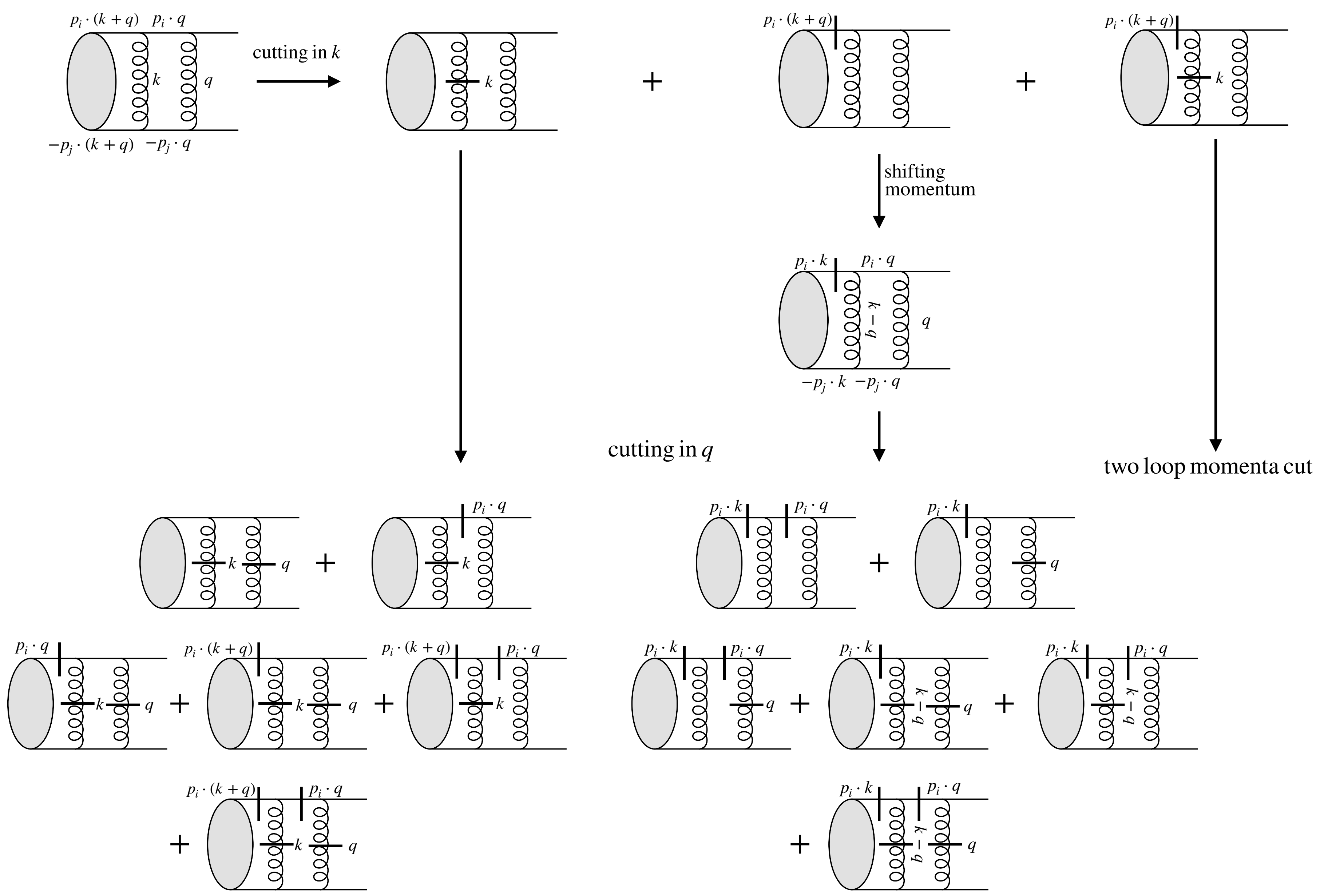
# Algebraic Problems

[Plätzer, Ruffa — arXiv:2012.15215]

Vital to the derivation and implementation of the algorithm:
Express virtual corrections as phase-space type integrals.

Cutting algorithm and colour structures automated in Mathematica.

Need to **generalise this to the two-loop case**,
breakdown to match with real emission momentum flow.



Feynman tree theorem:

$$\frac{1}{[q^2 - i0(T\cdot q)|T\cdot q|]} = \frac{1}{[q^2 + i0(T\cdot q)^2]} + 2\pi i\delta(q^2)\theta(T\cdot q)$$

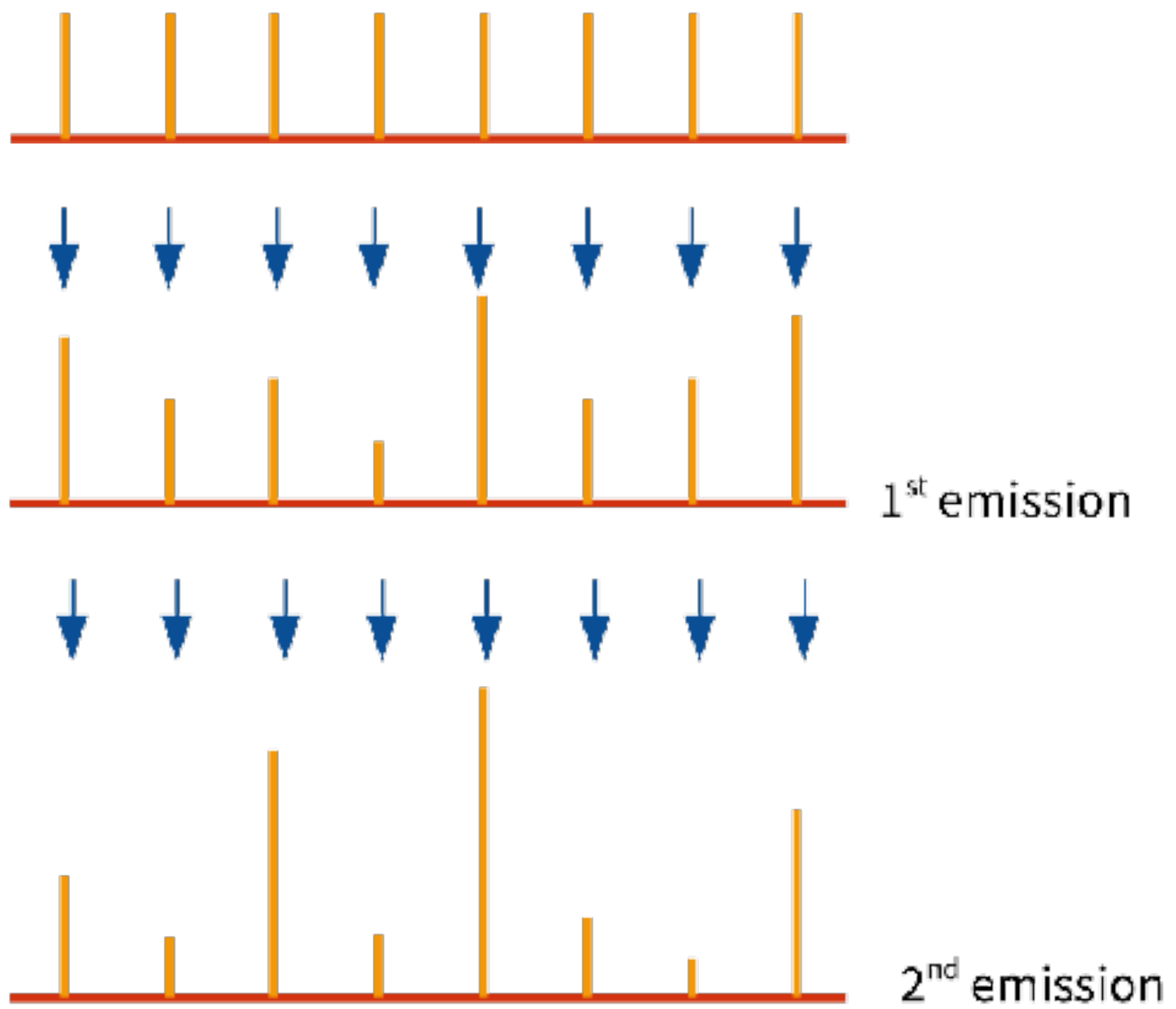
Extend to Eikonal and higher-power propagators:

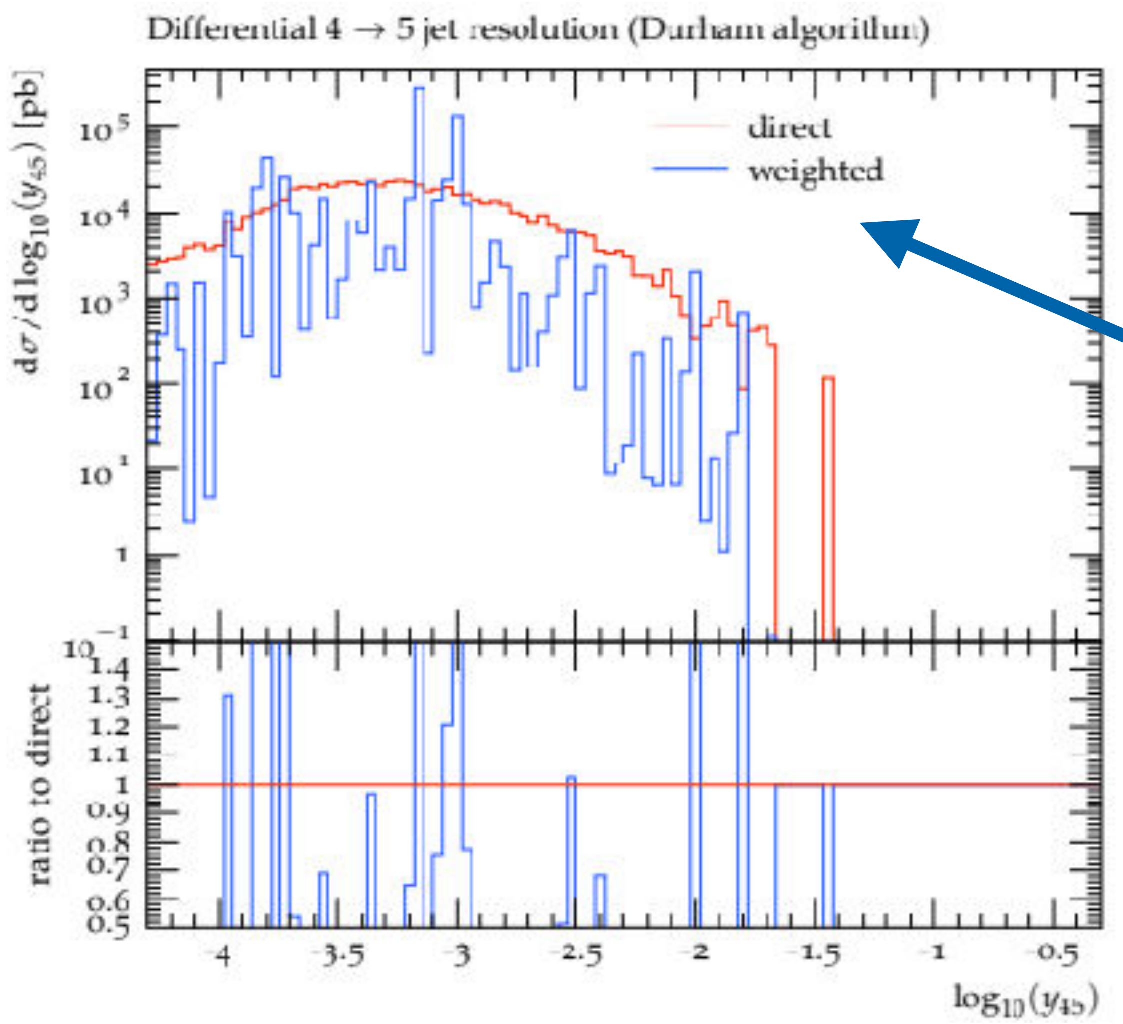
$$\frac{1}{2p_i\cdot k - i0(T\cdot p_i)^2} = \frac{1}{2p_i\cdot k + i0(T\cdot p_i)^2} + 2\pi i\ \delta(2p_i\cdot k)$$

$$\frac{1}{[q^2 - i0(T\cdot q)|T\cdot q|]^2} - \frac{1}{[q^2 + i0(T\cdot q)^2]^2} = -2i\pi\theta(T\cdot q)\delta'(q^2)$$

# Weighted Veto Algorithms & Resampling

[Olsson, Plätzer, Sjödahl — EPJ C80 (2020) 10, 934]

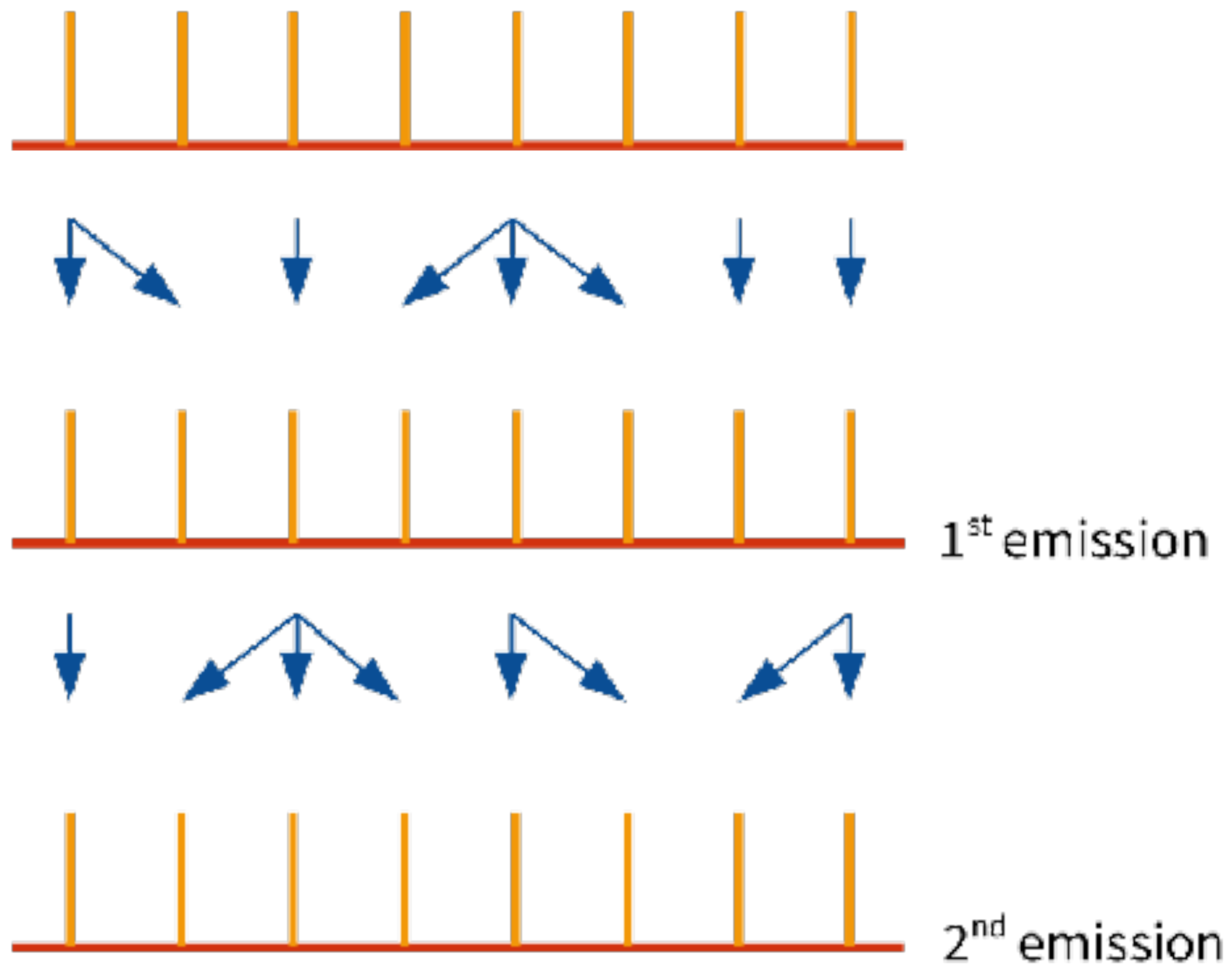


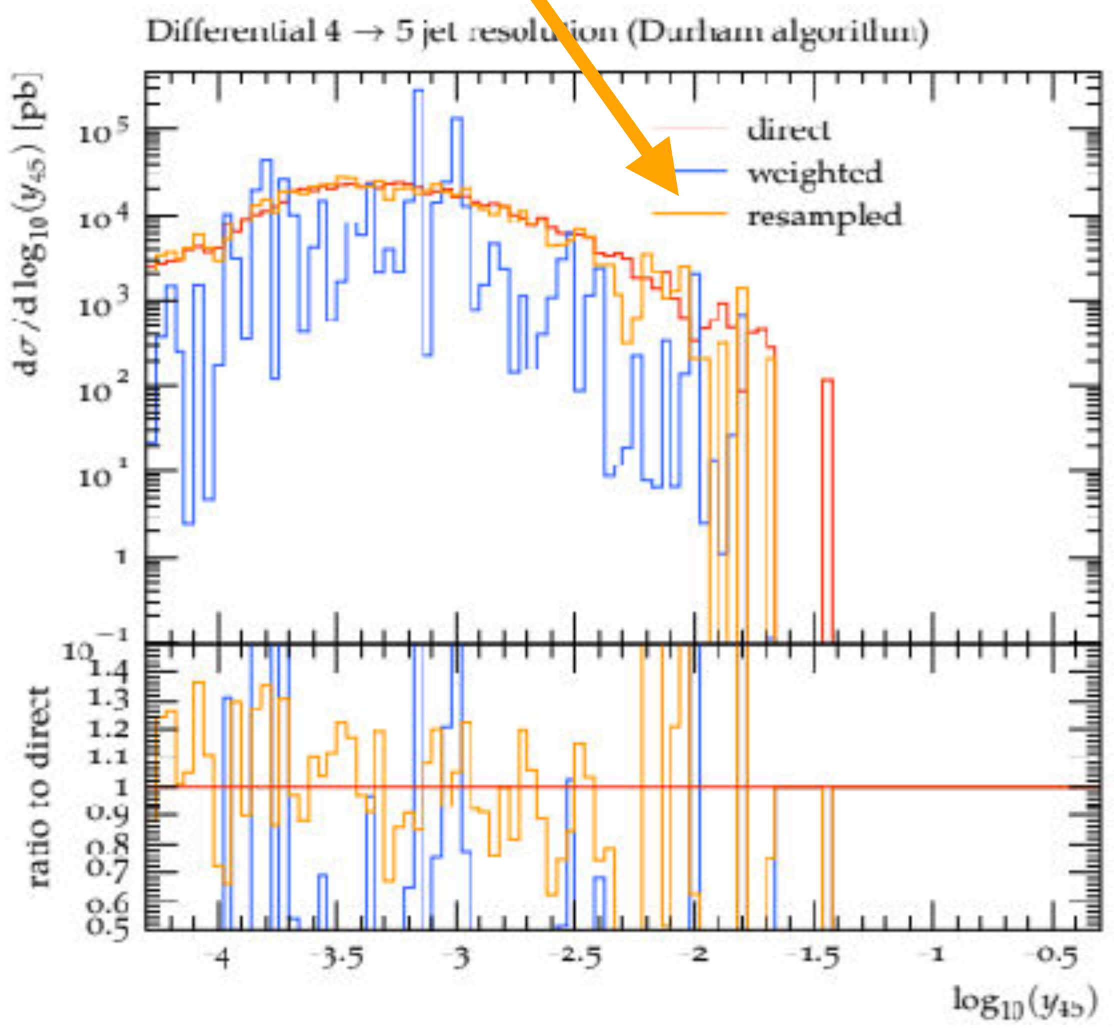




Weighted branching algorithms exhibit prohibitive weight distributions & convergence issues.

Result without resampling

Result with resampling



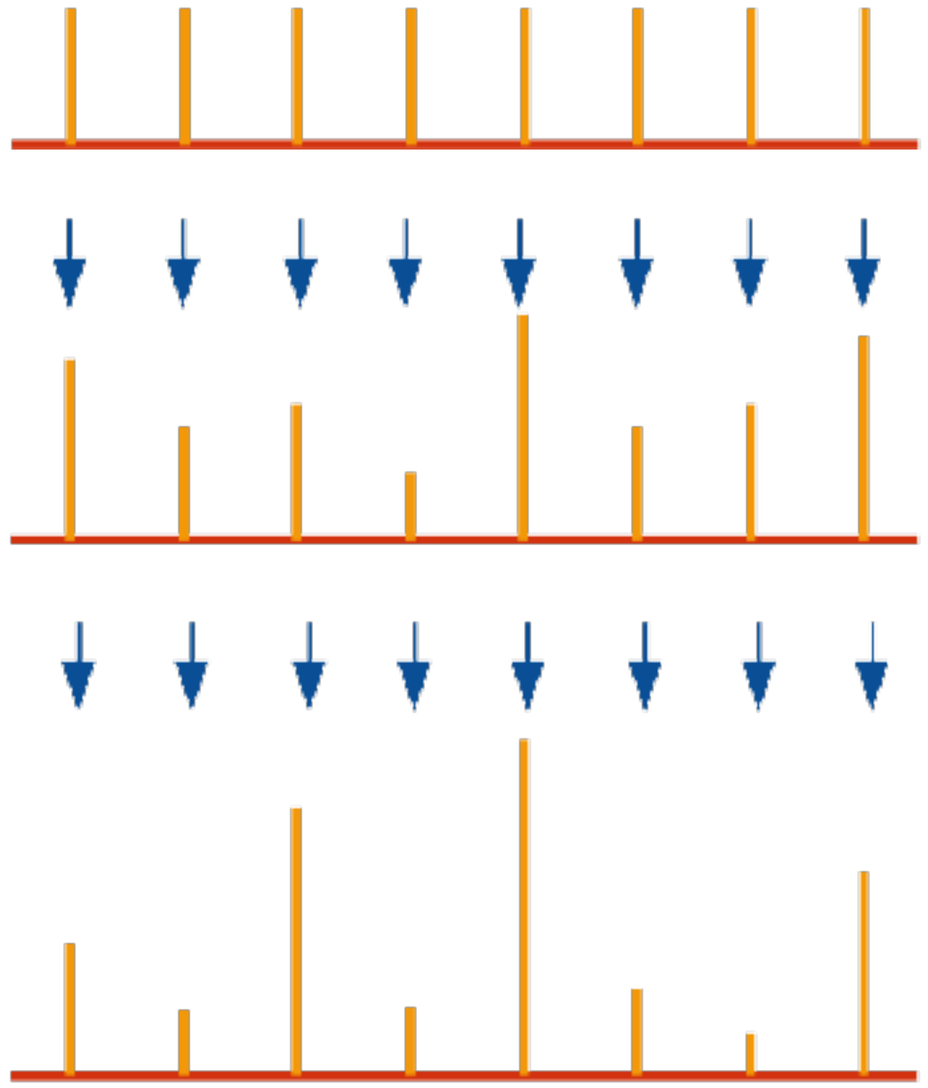

Resampling algorithms can compress weight distributions at intermediate steps.

Interdisciplinary exchange!

Python toolbox developing.

# Weighted Veto Algorithms & Resampling

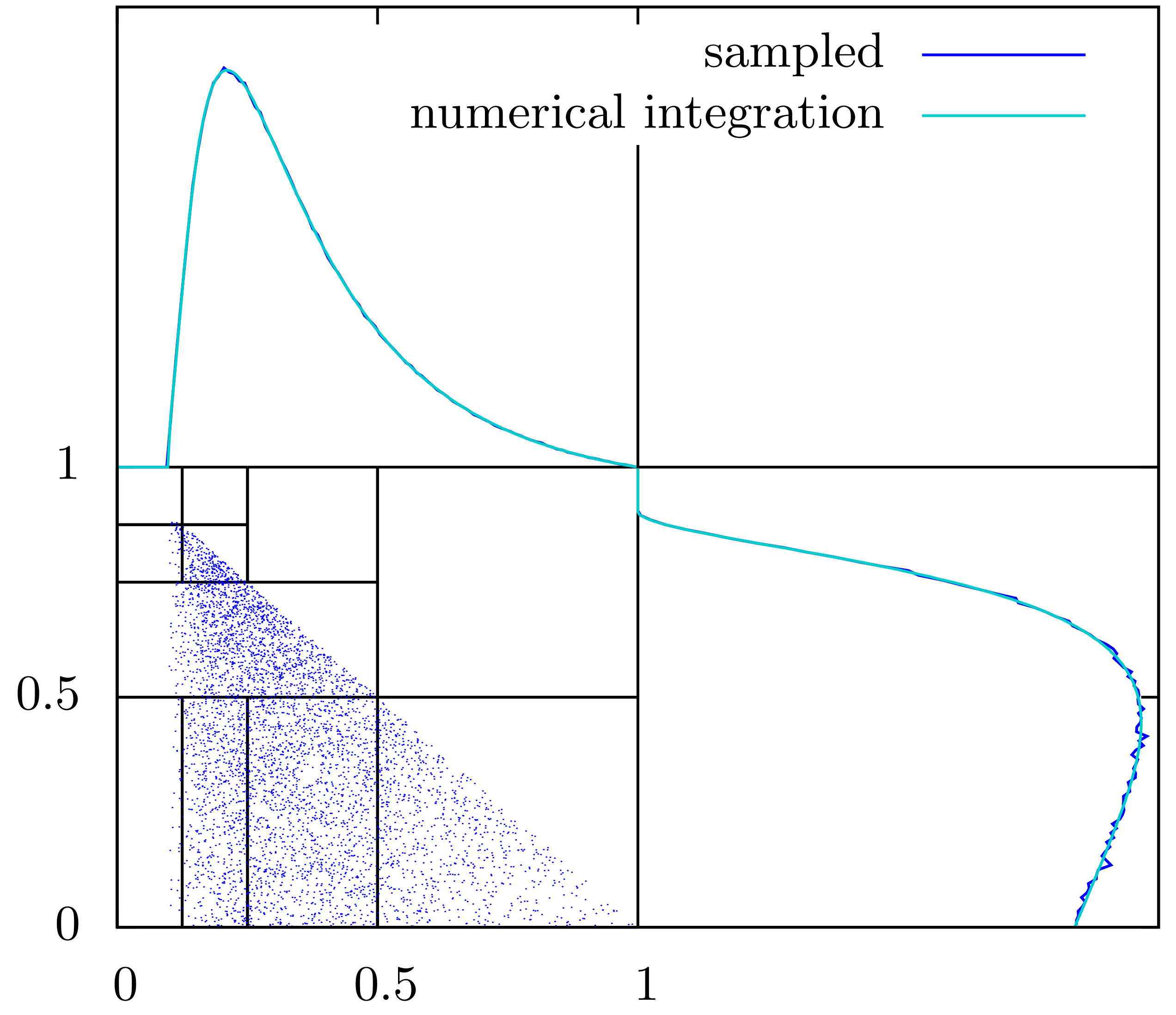
[Olsson, Plätzer, Sjödahl — EPJ C80 (2020) 10, 934]

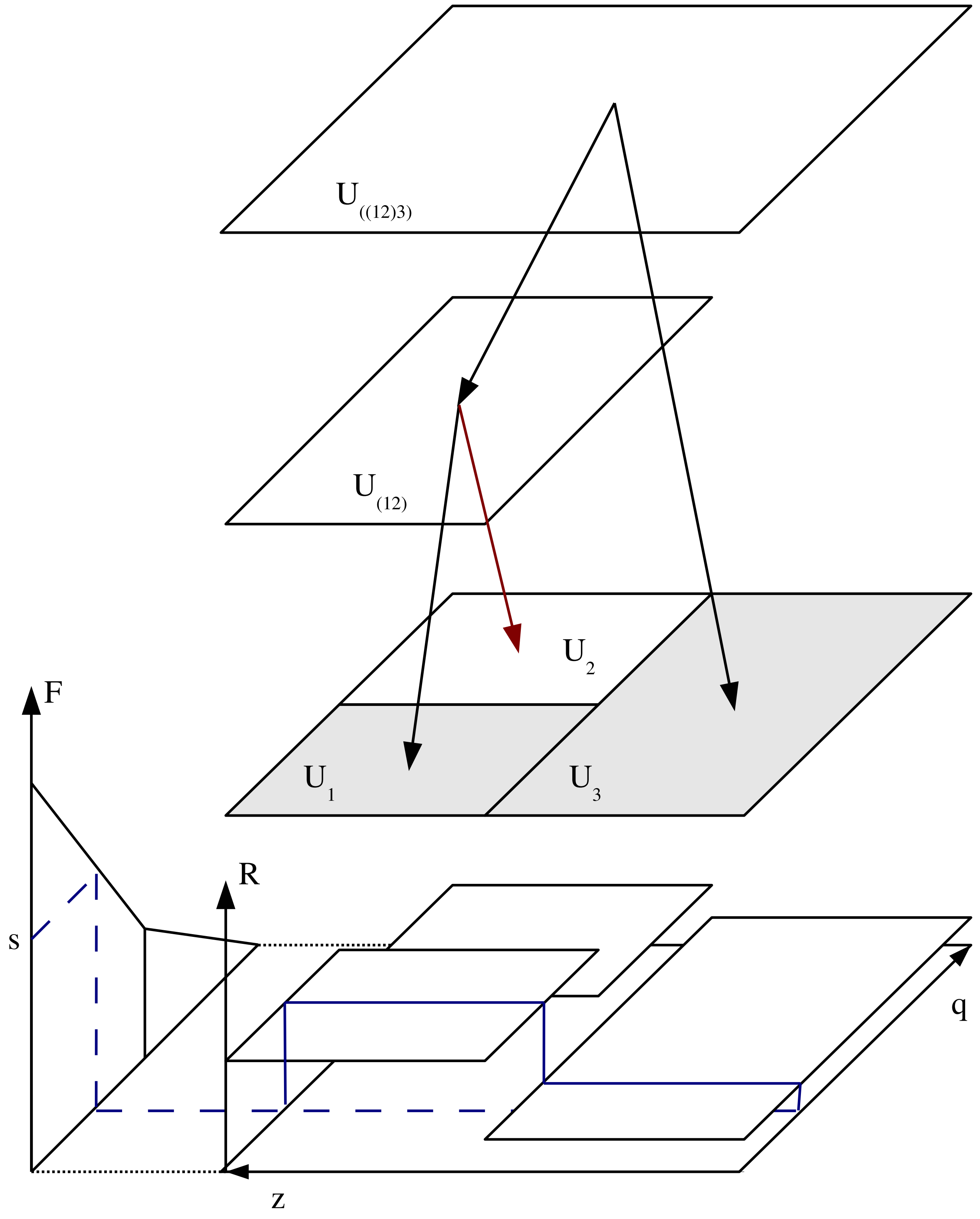


…ibitive
…issues.

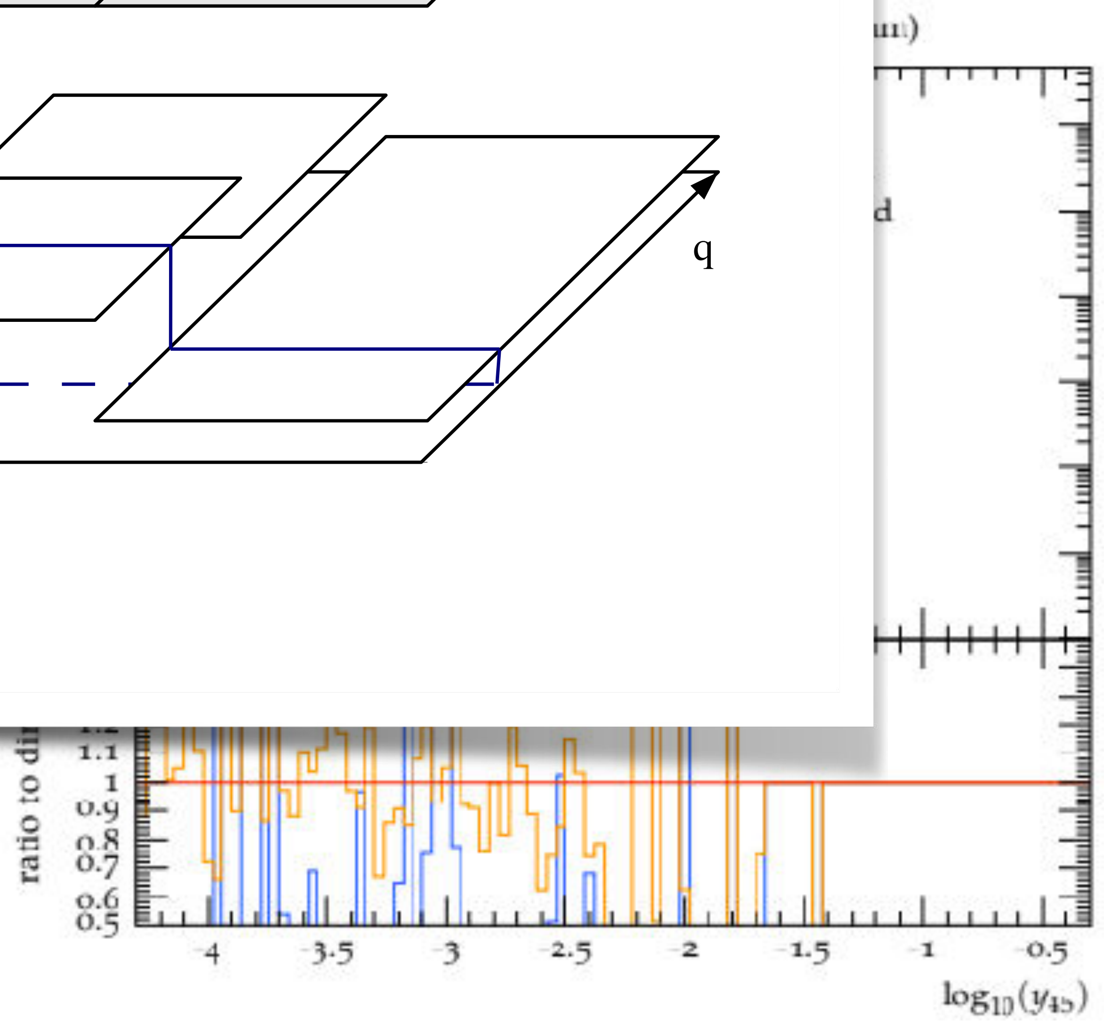
Combine with adaptive MC methods
for sampling shower evolution.

[Plätzer — EPJ C 72 (2012) 1929]

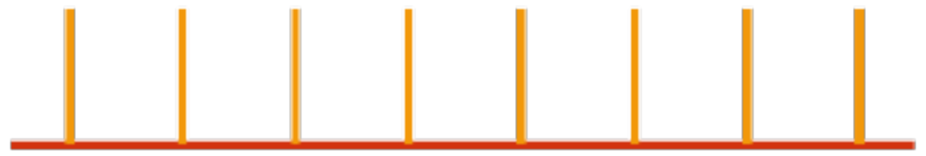


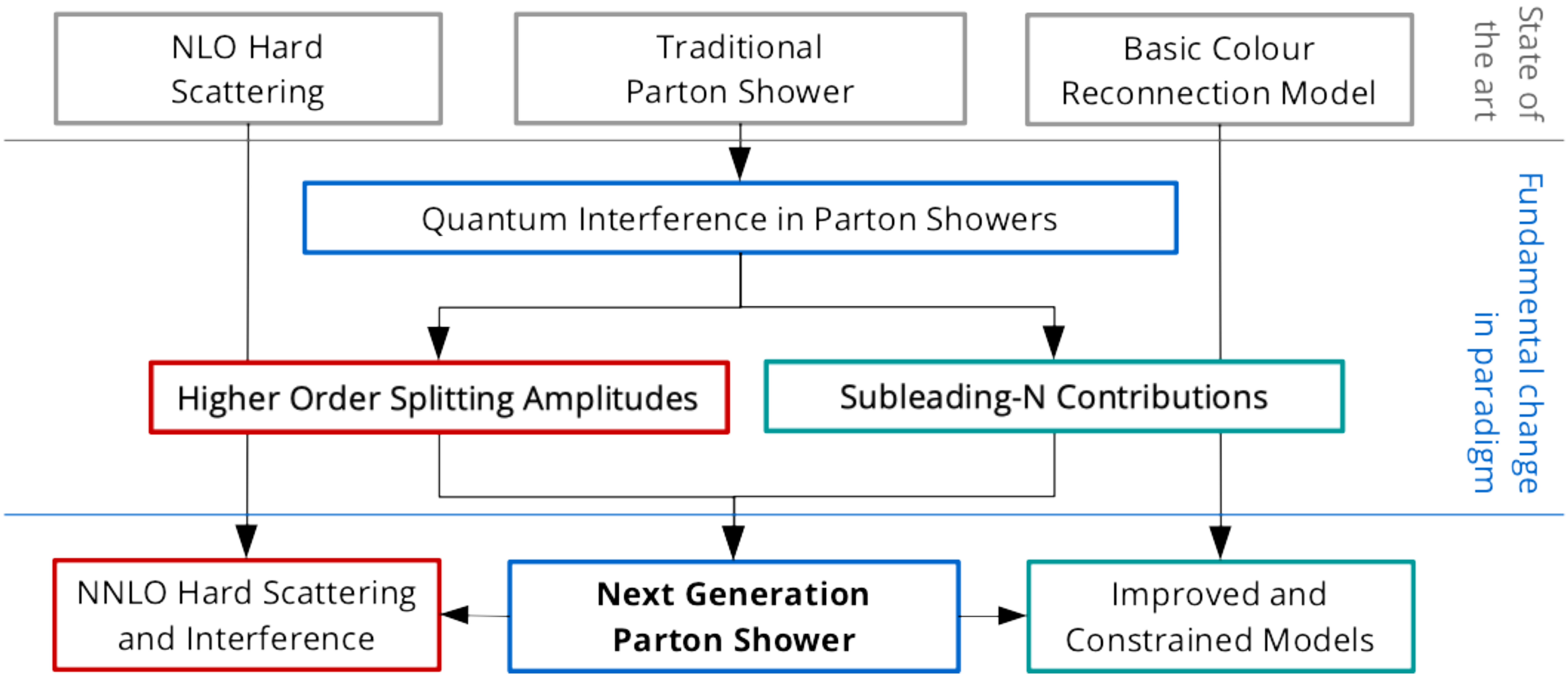

Resampling algorithms…
distributions at interm…



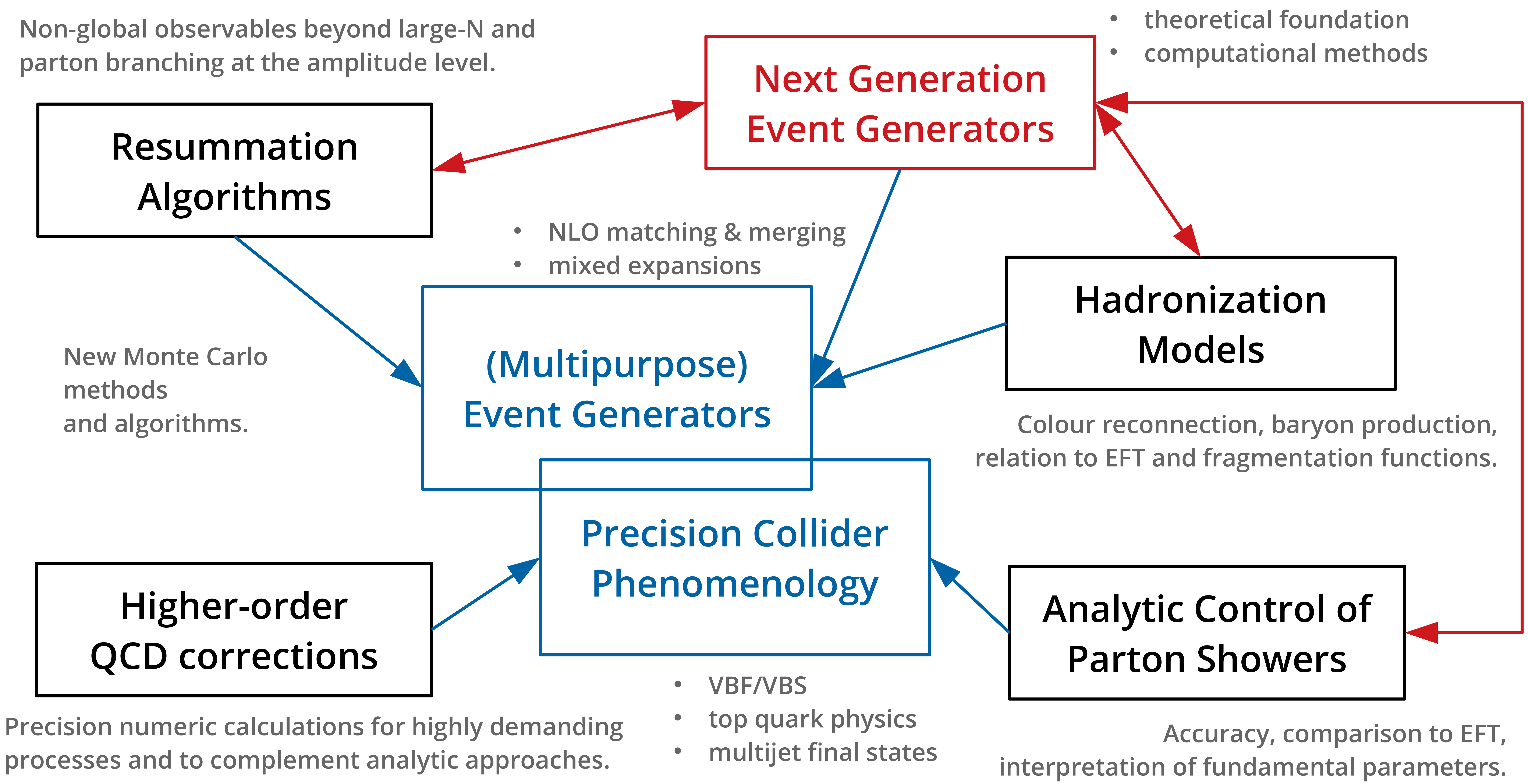
Interdisciplinary exchange!
Python toolbox developing.



# Foundations, Tools & Phenomenology



# Foundations, Tools & Phenomenology




**Computational tools for QFT and simulations** will always be vital to phenomenology.
**Algorithms, computing & contact to experiments** always go hand in hand.
Applications could range from colliders to cosmic rays to dark matter or neutrino physics.

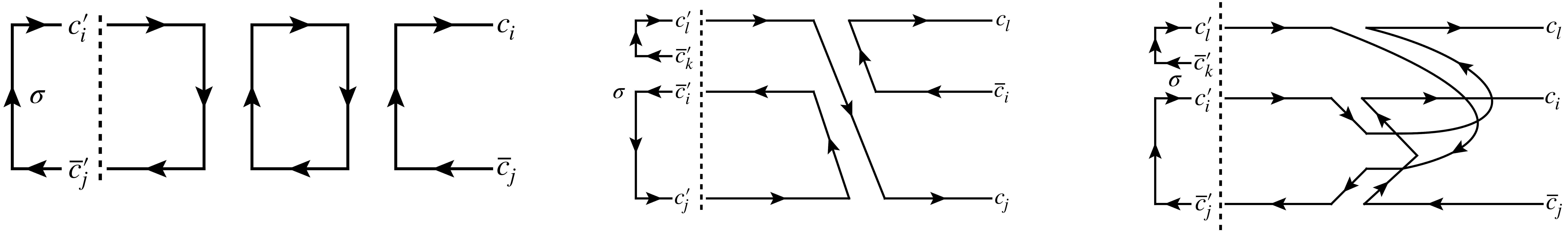
# Thank you!

# Going to Higher Orders

Anomalous dimension at two loops:

[Plätzer, Ruffa — arXiv:soon]

$$[\tau|\mathbf{\Gamma}|\sigma\rangle = (\alpha_s N)[\tau|\mathbf{\Gamma}^{(1)}|\sigma\rangle + (\alpha_s N)^2[\tau|\mathbf{\Gamma}^{(2)}|\sigma\rangle + \ldots$$



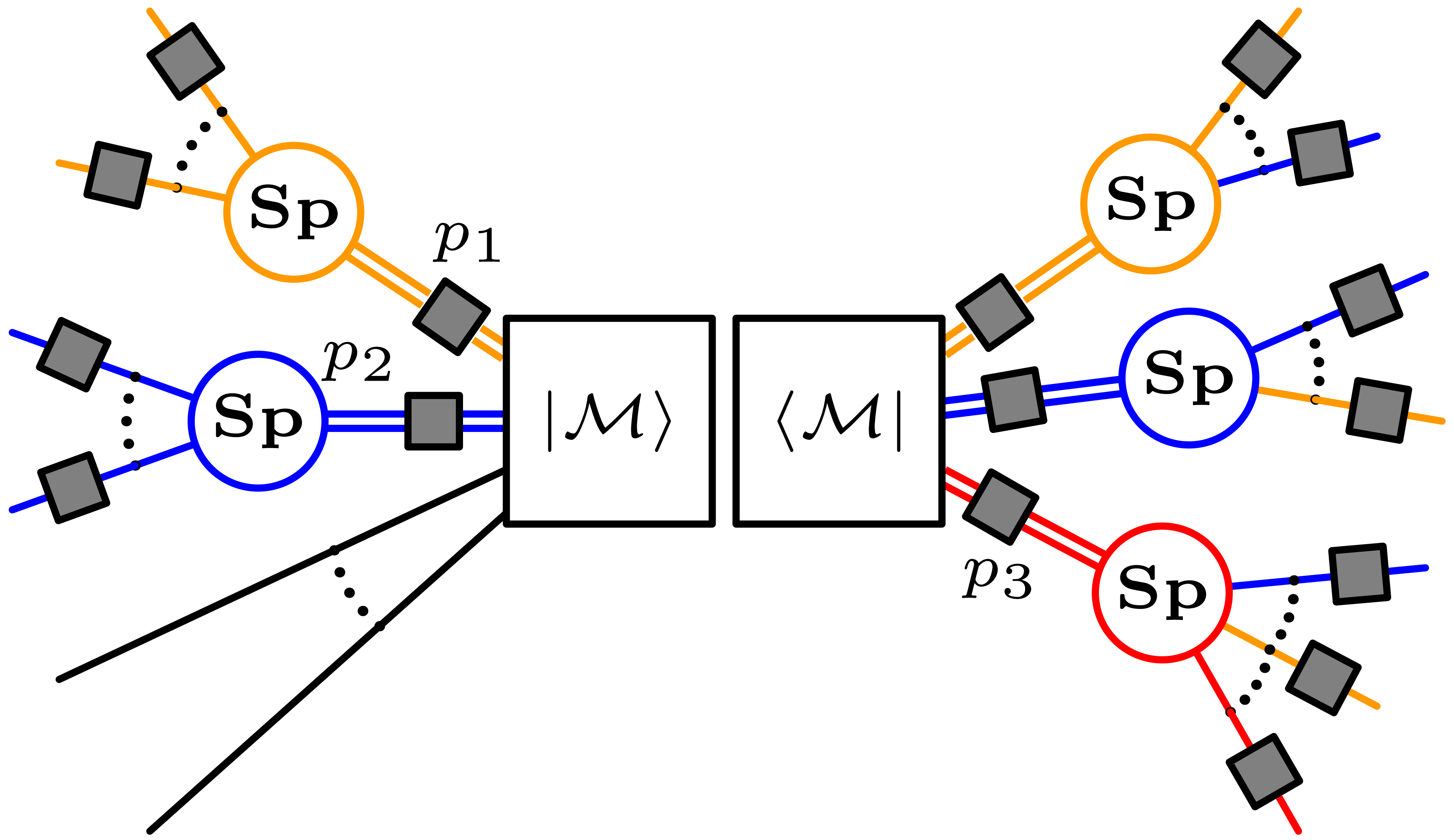

**Colour structures imply colour-diagonal three parton correlations:** Dipoles are not enough!

$$[\tau|\mathbf{\Gamma}^{(2)}|\sigma\rangle = \left(\Gamma^{(2)}_\sigma + \frac{1}{N^2}(\rho_\sigma + \tilde{\rho}) + \frac{1}{N^4}\rho^{(2)}\right)\delta_{\sigma\tau}$$
$$+ \frac{1}{N}\left(\Sigma^{(2)}_{\sigma\tau} + \hat{\Sigma}^{(2)}_{\sigma\tau}\right) + \frac{1}{N^3}\tilde{\Sigma}^{(2)}_{\sigma\tau} + \frac{1}{N^2}\left(\Sigma'^{(2)}_{\sigma\tau} + \Sigma''^{(2)}_{\sigma\tau}\right)$$

# Novel Calculational Techniques

[Löschner, Plätzer, Simpson — in preparation]

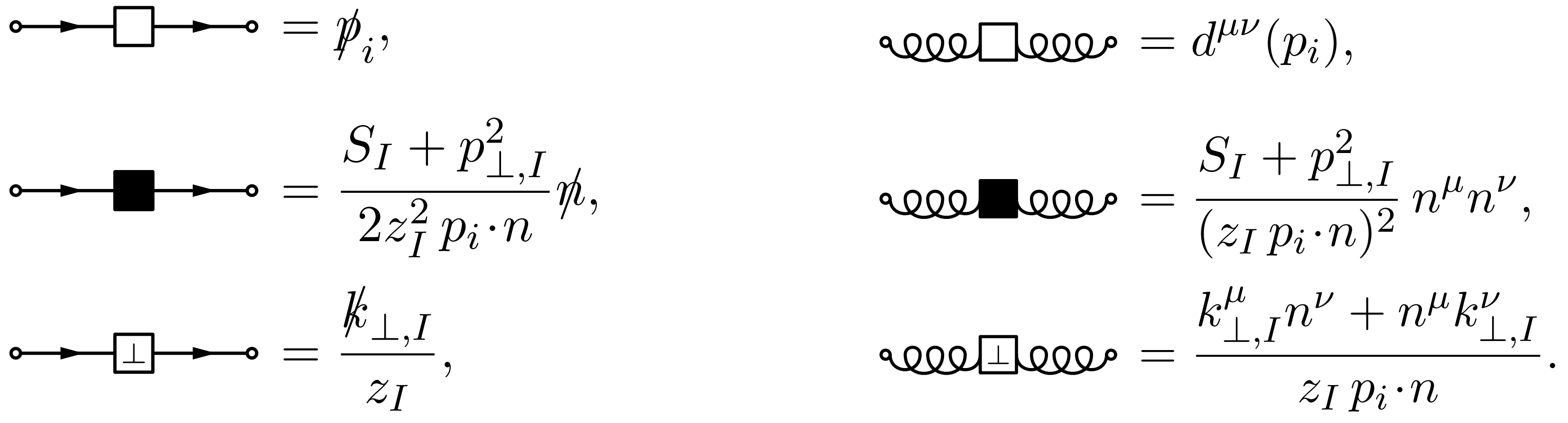
Extend double real emission beyond the double-soft case.

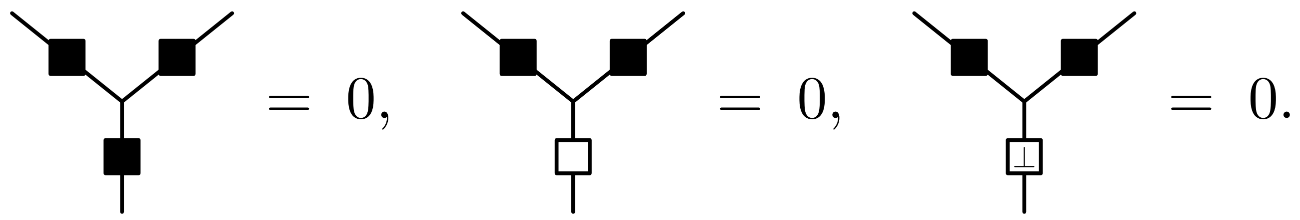



Recoil treated in sync with the factorisation and iteration of the splitting kernels.

Systematic underlying power counting — could even allow for subleading power expansions.

Disentangle different collinear sectors, use effective set of Feynman rules within physical gauge.

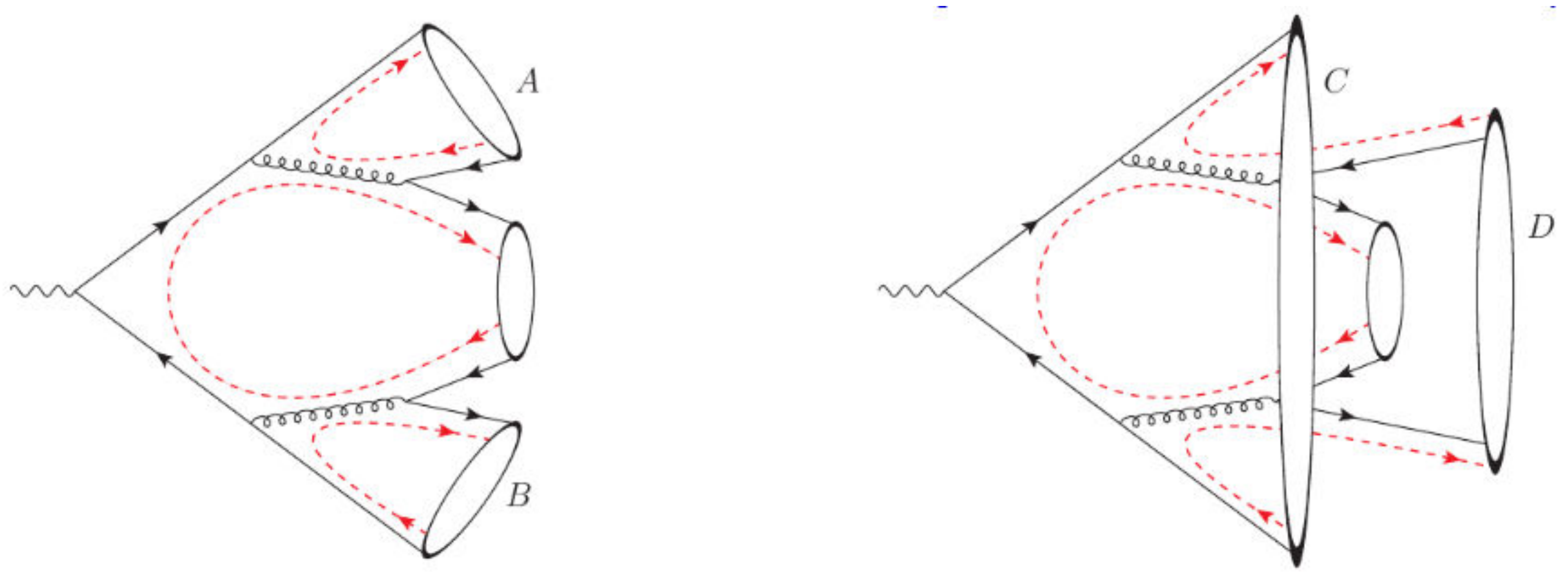


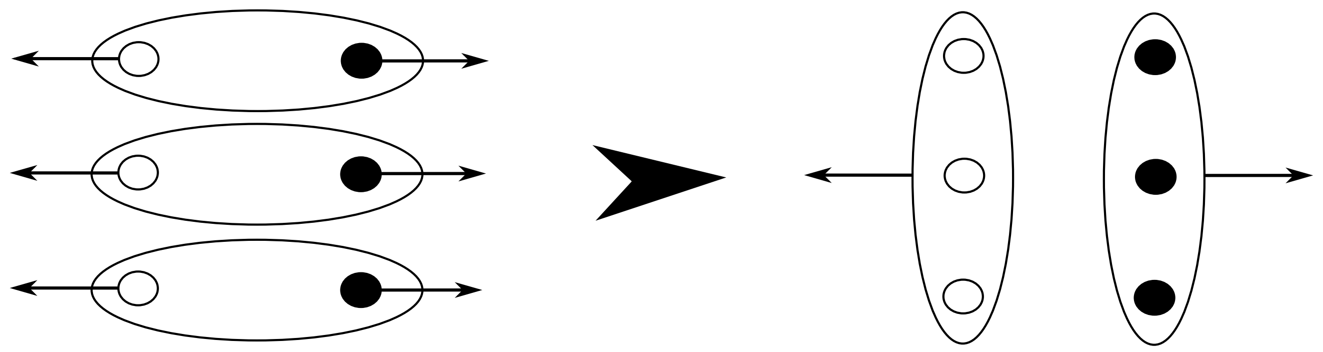

Connection to SCET?

# Colour Reconnection & Hadronization

Cluster re-wiring based on geometric criterion including Baryonic reconnection.




$$R_{q,qq} + R_{\bar{q},\bar{q}\bar{q}} < R_{q,\bar{q}} + R_{qq,\bar{q}\bar{q}}$$

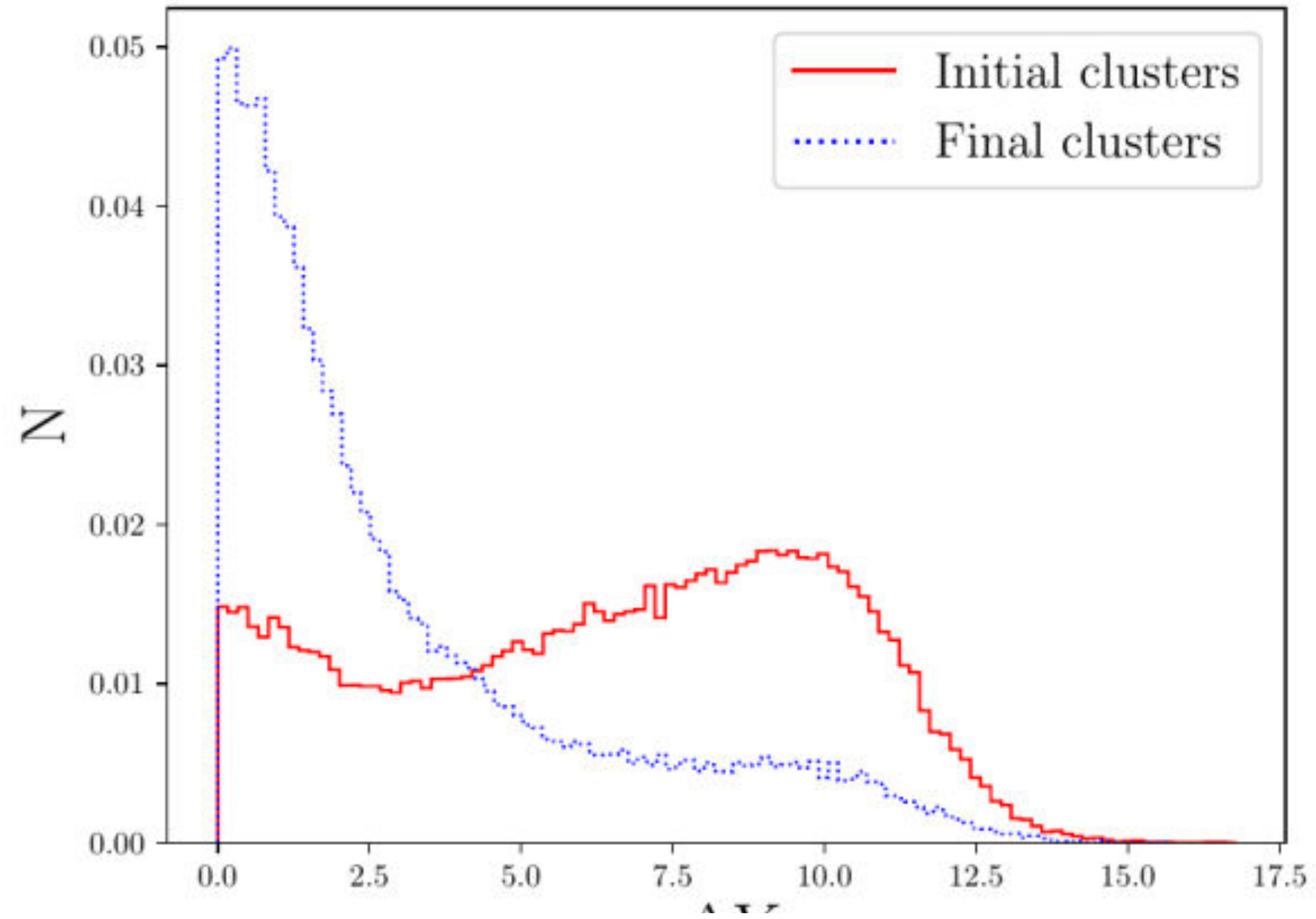


Approach colour reconnection from colour evolution: perturbative component?

Reconnection amplitude

$$\mathcal{A}_{\tau\to\sigma} = \langle\sigma|\mathbf{U}\left(\{p\},\mu^2,\{M_{ij}^2\}\right)|\tau\rangle$$

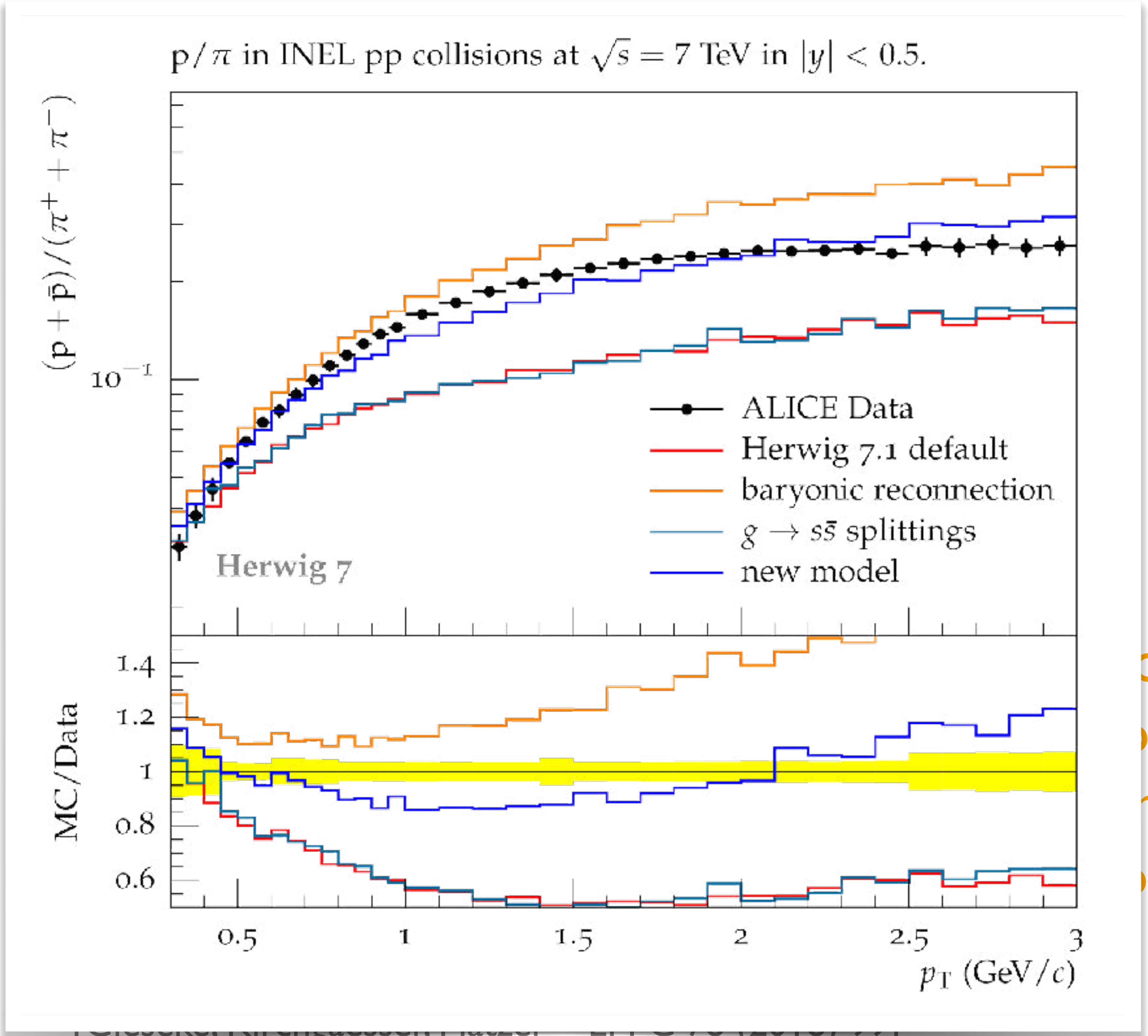
Strong support for geometric models from perturbative evolution.




[Gieseke, Kirchgaesser, Plätzer – EPJ C 78 (2018) 99]

[Gieseke, Kirchgaesser, Plätzer, Siodmok – JHEP 11 (2018) 149]

# Colour Reconnection & Hadronization

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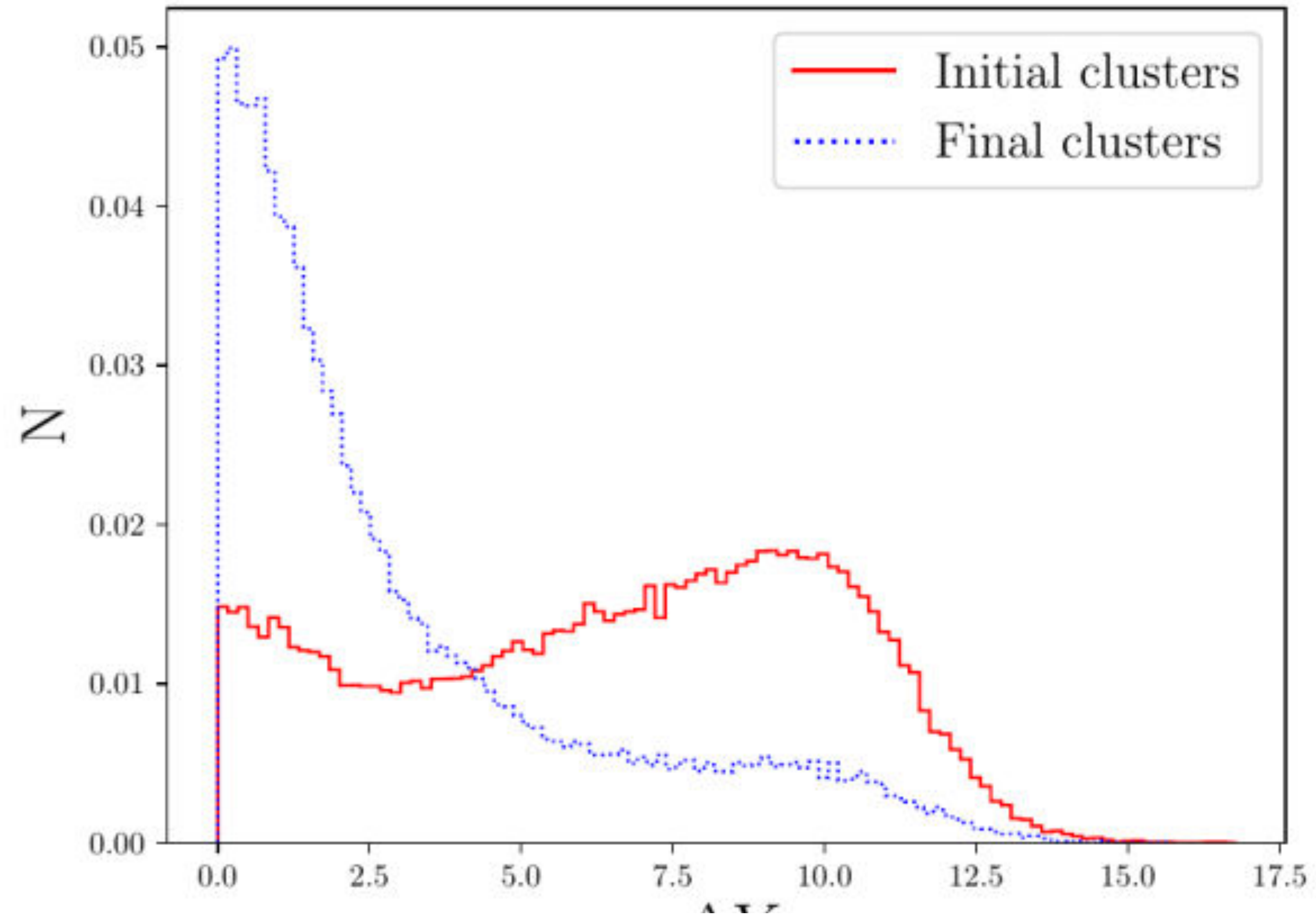


[Gieseke, Kirchgaesser, Plätzer, Siodmok – JHEP 11 (2018) 149]