Simon Plätzer Institute of Physics — NAWI, University of Graz Particle Physics — University of Vienna

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Thomas Rath - Institute for Chemistry and Technology of Materials (ICTM), NAWI Graz, Graz University of Technology, Graz 8010, Austria; o orcid.org/0000-0002 4837-7726; Email: thomas.rath@tugraz.at

Synthesis of Enantiopure Sulfoxides by Concurrent Photocatalytic Oxidation and Biocatalytic Reduction

Sarah Bierbaumer, Dr. Luca Sch mund, Alexander List, Dr. Christoph K. Winkler 🔀 Dr. Silvia M. Glueck 🔀 Prof. Dr. Wolfgang Kroutil







TU Graz



How do we accurately describe details of final states? How do we quantify precision in a comprehensive manner?

Matching beyond NLO QCD? Solve shower bottlenecks first?

How to benchmark precision of QCD algorithms? How to accurately include EW and QED?

How to constrain hadronization models? What is their response to perturbative variations?

$d\sigma \sim L \times d\sigma_H(Q) \times PS(Q \rightarrow \mu) \times MPI \times Had(\mu \rightarrow \Lambda) \times ...$









Perturbative precision is far from the last word:

E.g. lack of understanding of baryon production is limiting the power of q/g discrimination.

[see also Siodmok's talk]

Personal selection of some recent topics: Parton showers, hadronization and their interface. And new algorithms.

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deviation of reconstructed pt



simulated pt

[ATLAS-PUB-2022-021]

 $d\sigma \sim L \times d\sigma_H(Q) \times PS(Q \rightarrow \mu) \times MPI \times Had(\mu \rightarrow \Lambda) \times ...$

Shower & Parton Branching Paradigms



Parton branchings order in angle.



- Recoil global
- Links to analytic use of coherent branching



Sequences of emission scales and momentum fractions as Markov process. Restore momentum conservation per emissions or at end of evolution.

$$dS = \frac{\alpha_s}{2\pi} \frac{d\tilde{q}_i^2}{\tilde{q}_i^2} dz P(z_i) \exp\left(-\int_{\tilde{q}_i^2}^{Q^2} \frac{dq^2}{q^2} \int_{z_-(k^2)}^{z_+(k^2)} d\xi \frac{\alpha_i}{2}\right)$$

emission rate



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Dipole branchings order in transverse momentum.

- Driven by large-N dipole ulletpattern and colour flows
- Momentum conservation for each emission
- Advantageous for matching & merging

Herwig 7, Pythia 8, Sherpa, PanScales, Deductor

k $l \leq 2k$





no emission probability



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

LHC-age Working Horses

	Current release series	Hard matrix elements	Shower algorithms	NLO Matching	Multijet merging	MPI	Hadronization	Shower variation
H7	Herwig 7	Internal, libraries, event files	QTilde, Dipoles	Internally automated	Internally automated	Eikonal	Clusters, (Strings)	Yes
CEP	Pythia 8	Internal, event files	Pt ordered, DIRE,VINCIA	External	Internal, ME via event files	Interleaved	Strings	Yes
	Sherpa 2	Internal, libraries	CSShower, DIRE	Internally automated	Internally automated	Eikonal	Clusters, Strings	Yes

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r ns	



Global event shapes from coherent branching

LL — qualitative

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$H(\alpha_s) \times \exp\left(Lg_1(\alpha_s L) + \frac{g_2(\alpha_s L)}{g_2(\alpha_s L)} + \frac{\alpha_s g_3(\alpha_s L)}{g_3(\alpha_s L)} + \dots\right)$

NLL — quantitative NNLL — precision



 $\alpha_s L \sim 1$



Non-global observables in the large-N limit Global event shapes from coherent branching, subject from dipole branching to appropriate initial conditions:



[Catani, Trentadue, Webber, Marchesini]

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$$\frac{\partial G_{ab}(t)}{\partial t} = -\int_{\text{in}} \frac{\mathrm{d}\Omega_k}{4\pi} \omega_{ab}(k) G_{ab}(t) + \int_{\text{out}} \frac{\mathrm{d}\Omega_k}{4\pi} \omega_{ab}(k) \Big[G_{ak}(t) G_{kb}(t) - \frac{\mathrm{d}\Omega_k}{4\pi} \Big] \Big] d\Omega_k + \int_{\text{out}} \frac{\mathrm{d}\Omega_k}{4\pi} \Big] d\Omega_k + \int_{\text{out}} \frac{$$

[Banfi, Marchesini, Smye — JHEP 08 (2002) 006]









(N)NLO with matching

NLL with coherent branching Issues in dipole showers

Can we push this to NLL_{global} / LL_{non-global} in one (dipole) algorithm?

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Issues in coherent branching LL with dipole showers

 $\alpha_s L \sim 1 \quad \alpha_s N^2 \sim 1$



Can we push this to NLL_{global} / LL_{non-global} in one (dipole) algorithm?

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Based on amplitude

evolution

Demonstrate NLL accurate evolution:

• PanScales — numerical

[PanScales — Dasgupta, Monni, Salam, Soyez +]

[Nagy, Soper]

• Forshaw/Holguin/Plätzer — analytical

[aim at improving Herwig 7 dipole shower] • Sherpa — numerical/analytical

[Herren, Höche, Krauss, Reichelt, Schönherr]

 $\alpha_s L \sim 1 \qquad \alpha_s N^2 \sim 1$

NLLglobal/LLnon-global showers

Two main ingredients in intricate interplay with ordering variable:



Implementations now in Deductor, Herwig, PanScales, Sherpa

Not only present in dipole showers, can even aff coherent branching $A_{4 \text{ jet}+(g)}|_{1||4} \approx \frac{2\alpha_s}{\pi} \int_{0}^{1} (4)S_1^{2,3}\Theta(\theta_{15} < \theta_{14})|1 \cdot 1|_4 + \frac{4}{3}S_2^{1,3}|2 \cdot 1|_4 + \frac{4}{3}S_2^{1,3}|2 \cdot 1|_4$ [Bewick, Ferrario, Richardson, Seymour —JHEP 04 (2020) 019] ${}^{(4)}S_4^{1,2}|4\cdot 4|_4 + {}^{(4)}S_1^{2,3}\Theta(\theta_{15} > \theta_{14})|1 +$



Can extent this to three jet topologies:

$$^{(n-1)}\mathbf{S}_{i}^{j,k} = rac{1}{2} \left(\omega_{ij} + \omega_{ik} - \omega_{jk}\right)$$

$$\begin{aligned} & \cdot 2|_{4} + {}^{(4)}\mathrm{S}_{3}^{1,2}|_{3} \cdot 3|_{4} + & \left[i \cdot j\right] = \mathbf{T}_{i} |M_{n-1}\rangle \langle M_{n-1}|_{4} \mathbf{T}_{j}^{\dagger} \\ & \quad \mathrm{Holguin, Forshaw, Platzer} - \mathrm{HEP} \, \mathrm{OS} \, (2022) \\ & \quad + 4 \cdot 1 + 4|_{4} \end{bmatrix} \cdot & \sum_{j} \mathbf{T}_{j} = \mathbf{0} \quad \omega_{ij}(q_{n}) = \frac{q_{i} \cdot q_{j}}{q_{n} \cdot q_{i} \, q_{n} \cdot q_{j}} \end{aligned}$$





Where it (also) matters

Coherent branching jet mass including mass effects:

$$z(1-z)\tilde{q}^{2} = -m_{\tilde{i}\tilde{j}}^{2} + \frac{m_{i}^{2}}{z} + \frac{m_{j}^{2}}{1-z} - \frac{p_{\perp}^{2}}{z(1-z)}$$

using [Gieseke, Stephens, Webber – JHEP 0312 (2003) 045]

NLL accurate for global observables with massive quarks.

Top mass definition from
coherent branching. $m_t^{\rm MC} =$
 $m_t^{\rm CB}(Q)$ [Hoang, Plätzer, Samitz — [HEP 1810 (2018) 200] $m_t^{\rm CB}(Q)$

Take home message: hadronization and mass scheme compensate for shower cutoff dependence.

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 $m_t^{\rm MC} = m_t^{\rm pole} + \Delta_m^{\rm pert} + \Delta_m^{\rm non-pert}$

$$_{0}) = m_{t}^{\text{pole}} - \frac{2}{3}Q_{0} \alpha_{s}(Q_{0}) + \mathcal{O}(\alpha_{s}^{2})$$



Showers at higher orders

Identifying algorithms for higher order parton shower kernels is an active field.

- How to remove iterated pieces?
- How is the large-N limit working?
- How to combine soft and collinear regions?

Towards second-order showers: unordered contributions

- $\bullet\,$ sector showers allow to include direct $2 \rightarrow 4$ branchings in a simple way
- divide phase space into strongly-ordered and unordered region
 - s.o. region: only single-unresolved limits
 - u.o. region: only double-unresolved limits
- $2 \rightarrow 4$ branchings important ingredient to NNLO+PS $(+ \text{ virtual corrections to } 2 \rightarrow 3)$

[C. Preuss for Vincia — PSR 21]



[Dulat, Höche, Prestel — Phys.Rev.D 98 (2018) 7] [Gellersen, Höche, Prestel — Phys.Rev.D 105 (2022) 11]











[Plätzer, Ruffa — JHEP 06 (2021) 007] [Löschner, Plätzer, Simpson — arXiv:2112.14454]

> $z_1 = (1-z)z_p$ $z_2 = (1-z)(1-z_n)$ $z_3 = z$

> > [Dasgupta, El-Menoufi — JHEP 12 (2021) 158]





Showers at higher orders

Identifying algorithms for higher order parton shower '

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Towards second-order showers: unordered contributions

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[Dasgupta, El-Menoufi — JHEP 12 (2021) 158]







Showering beyond QCD

First steps to extend showers from QCD to other interactions: [Herwig, Pythia, Sherpa provide QED and (some) EWK]

- Angular ordered shower in quasi-collinear limit rather straightforward.
- Relation to large-angle soft pattern and initial conditions still need investigation

Different charges require different angular ordering cones: one evolution variable per interaction.



How do we lift this to the same level of cornering QCD showers (and matching)?





Work ongoing, e.g. [Plätzer, Sjödahl — arXiv:2204.03258]

[Masouminia, Richardson — JHEP 04 (2022) 112]







Amplitude evolution

$$\mathbf{A}_n(q) = \int_q^Q \frac{\mathrm{d}k}{k} \, \mathrm{P}e^{-\int_q^k \frac{\mathrm{d}k'}{k'} \mathbf{\Gamma}(k')}$$

Markovian algorithm at the amplitude level: Iterate gluon exchanges and emission.

Different histories in amplitude and conjugate amplitude needed to include interference.

[Angeles, De Angelis, Forshaw, Plätzer, Seymour – JHEP 05 (2018) 044] [Forshaw, Holguin, Plätzer – JHEP 1908 (2019) 145, ...] [Nagy, Soper — PRD 98 (2018) 1, ...]







 $\mathbf{D}_n(k) \mathbf{A}_{n-1}(k) \mathbf{D}_n^{\dagger}(k) \overline{\mathbf{P}}e^{-\int_q^k \frac{\mathrm{d}k'}{k'} \mathbf{\Gamma}^{\dagger}(k')}$





Simulations beyond leading colour

CVolver solves evolution equations in colour flow space



Agrees with [Hatta et al. — Nucl.Phys.B 962 (2021) 115273] using equivalent Langevin formulation.

 ρ





[De Angelis, Forshaw, Plätzer — PRL 126 (2021) 11] [Plätzer – EP] C 74 (2014) 2907]

$$\mathbf{D}_n(k) \mathbf{A}_{n-1}(k) \mathbf{D}_n^{\dagger}(k) \overline{\mathbf{P}}e^{-\int_q^k \frac{\mathrm{d}k'}{k'} \mathbf{\Gamma}^{\dagger}(k')}$$



Amplitude evolution rapidly evolving:

- Inclusion of hard collinear contributions?
- Electroweak and QED effects?
- Higher order contributions?
- Hadronization?

Electroweak evolution requires isospin and chirality flows, and better handling of kinematics.



Leverage both as a theory tool to construct showers as well as algorithms in their own right. Only approach to consistently combine interference terms in the hard process with showering.





Re-arrange soft and collinear evolution [Forshaw, Holguin, Plätzer – JHEP 1908 (2019) 145, ...]

[Plätzer, Sjödahl — arXiv:2204.03258]





The interface to hadronization



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[Bellm, Lönnblad, Plätzer, Prestel, Samitz, Siodmok, Hoang — Les Houches 2017]

The interface to hadronization

How do we consistently hadronize in light of (improved) shower algorithms? How to do this at subleading N and higher order shower evolution?





Implies evolution equations for both shower (amplitude) evolution as well as for a hadronization model.

> ecceccec eccecco 000000000

e.g. colour reconnection *implied* just as observed in [Gieseke, Kirchgaesser, Plätzer – EPJ C 78 (2018) 99] [Gieseke, Kirchgaesser, Plätzer, Siodmok – JHEP 11 (2018) 149]





μs

The interface to hadronization



construct by cutoff response

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[Plätzer – arXiv:2204.06956] plus work in progress

Stepping stone: match clusters to shower

UV limit of hadronization needs to reproduce soft limit of (angular ordered) shower.



figures by Daniel Samitz



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[Hoang, Plätzer, Samitz — in progress] [Kiebacher, Plätzer, Priedigkeit — in progress]

Tuning and hadronization corrections

Significantly different shapes of hadronization corrections (extracted bin by bin from Herwig)









C parameter parton versus hadron level

[Hoang, Plätzer, Samitz — in progress]

Tuning and hadronization corrections

Significantly different shapes of hadronization corrections (extracted bin by bin from Herwig)





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Hidden valley hadronization

Hidden valley angular ordered shower, based on new shower interactions framework



Herwig package complementing Pythia's hidden valley model. Blindly relying on validity of coherence and quasi-collinear limit ... among many other questions.

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More flexible cluster hadronization

[Kulkarni, Masouminia, Papaefstathiou, Plätzer, Siodmok, Stafford — in progress]







Algorithms & Efficiency

Sudakov-type densities central to Showers



Negative P or unknown overestimate requires weighted veto algorithm, with in principle arbitrary proposal kernel and veto probability.

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[Olsson, Plätzer, Sjödahl — EPJC 80 (2020) 10] [Plätzer, Sjödahl — EP] Plus 127 (2012) 26] $Q' \leftarrow Q, w \leftarrow w_0$ loop A trial splitting scale and variables, q, z, are generated according to $S_R(q|Q', z, x)$, for example using Alg. 1. if $q = Q_0$ then There is no emission and the cut-off scale Q_0 is returned while the event weight is kept at w. else if $\mathbf{rnd} \leq \epsilon$ then The trial splitting variables q, z are accepted, and $w \leftarrow w \times \frac{1}{\epsilon} \times \frac{P(Q', z, x)}{R(Q', z, x)}.$ (3)else The emission is rejected, and the algorithm continues with $w \leftarrow w \times \frac{1}{1-\epsilon} \times \left(1 - \frac{P(q, z, x)}{R(q, z, x)}\right)$ $Q' \leftarrow q.$ (4)end if end if

end loop

















Weighted Veto Algorithms & Resampling



[Andersen, Gütschow, Maier, Prestel — EPJ C 80 (2020) 11]

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Some words on matching

Matching is important and challenging. NLO Matching & merging well established, can combine with NNLO and beyond using unitarized merging algorithms.

> [Plätzer — JHEP 08 (2013) 114] [Lönnblad, Prestel — JHEP 02 (2013) 049] e.g. N3LO — [Prestel — JHEP 11 (2021) 041]

True *matching* beyond NLO and including QED/EW needs much more progress on showers first.

Some progress towards NNLO by correcting showers. [Campbell, Höche, Li, Preuss, Skands — arXiv:2108.07133]

Showers need to demonstrate that their construction yields double emission kernels which read

> (2 correlated, ordered emissions) - (1x1 ordered emissions) + (2 correlated, un-ordered emissions)

> > [Plätzer – arXiv:2204.06956]

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Matching & merging has been focus of last decade.

Also for matching to more than NNLO QCD.

one of the main topics in the future, not only in light of measuring fundamental parameters.

Amplitude level evolution can serve as theoretical framework and algorithm in its own right.

We cannot argue that these effects are small if we do not have a tool to explicitly check.



- Multi-purpose event generators can start to do FCC physics, but a face a significant number of challenges.
- As we aim to use more and more of the complex structures, shower accuracy becomes the bottleneck.
- The understanding of hadronization effects and models, and their interplay with parton showers will be
- Need to explore subleading colour and other effects which are inaccessible to probabilistic algorithms:



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