

Fakultät Mathematik und Naturwissenschaften Institut für Kern- und Teilchenphysik

Modern event generation for the LHC

Features and caveats of the Sherpa event generator

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Introduction: Monte-Carlo event generators



- We want: Simulation of $pp \rightarrow$ full hadronised final state
- MC event representation (e.g. $pp \rightarrow t\bar{t}H$ event)
- We know from first principles:
 - Hard scattering at fixed order in perturbation theory
 - (Matrix Element)
 - Approximate resummation of QCD corrections to all orders (Parton Shower)
- Missing bits: Hadronisation/Underlying event (ignored today)



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Outline

- Introduction
- The parton shower approximation
- Correcting that approximation as far as possible:
 - NLO+PS matching (2002)
 - Tree-level ME+PS merging (2001)
 - ME+PS merging at NLO (2012)
- Practical considerations

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Perturbation Theory

- Cannot solve QCD and calculate $pp \rightarrow X$ exactly
- But can calculate parts of the perturbative series in *α_s*:



- Most precise calculations include $\mathcal{O}(\alpha_s^2)$ for some processes
- $\alpha_s^2 \approx 1\% \Rightarrow$ high enough precision, right?
- Why is that not always true?



- Predictions for inclusive observables calculable at fixed-order (~~ KLN theorem for cancellation of infrared divergences)
- But if not inclusive \rightarrow finite remainders of infrared divergences:

logarithms of
$$\frac{\mu_{\text{cut}}^2}{\mu_{\text{hard}}^2}$$
 with each $\mathcal{O}(\alpha_s)$

can become large and spoil convergence of perturbative series Examples:

- Study certain regions of phase space, like $p_{\perp}^Z \approx 0$ @ DY
- Making predictions for hadron-level final states: confinement at $\mu_{\rm had}\approx 1~{\rm GeV}$

\Rightarrow Need to resum the series to all orders

- Problem: We are not smart enough for that.
- Workaround: Resum only the logarithmically enhanced terms in the series
- \rightarrow Parton Showers!



Construction of a parton shower



Universal structure at all orders

• Factorisation of QCD real emission for collinear partons (*i*, *j*):

$${\cal R} \
ightarrow {\cal D}_{ij}^{({
m PS})} \equiv {\cal B} imes \left[8\pi lpha_s \ rac{1}{2 p_i p_j} \ {\cal K}_{ij}(p_i,p_j)
ight]$$



Factorisation of phase space element

$$\mathrm{d}\Phi_{\mathcal{R}} \ \rightarrow \ \mathrm{d}\Phi_{\mathcal{B}} \,\mathrm{d}\Phi_1 = \mathrm{d}\Phi_{\mathcal{B}} \,\mathrm{d}t \, rac{1}{16\pi^2} \,\mathrm{d}z \, rac{\mathrm{d}\phi}{2\pi}$$

with evolution variable $t~\sim~2p_ip_j~\sim~ heta_{ij},~k_{\perp}^{ij},~Q_{ij}$

- $\Rightarrow \text{ Differential branching probability: } d\sigma_{ij}^{(\text{PS})} \sim dt \frac{\mathcal{D}_{ij}^{(\text{PS})}}{\mathcal{B}} \sim \frac{dt}{t} \frac{\alpha_s}{2\pi} \mathcal{K}_{ij}$
 - $d\sigma_{ii}^{(PS)}$ is universal and appears for each emission
 - How do we get the resummed branching probability according to multiple such emissions?

 \rightarrow Analogy to evolution of ensemble of radioactive nuclei: Survival probability at time t_1 depends on decay/survival at times $t < t_1$



Radioactive decay

Constant differential decay probability

 $f(t) = \text{const} \equiv \lambda$

• Survival probability $\mathcal{N}(t)$

$$-\frac{\mathrm{d}\mathcal{N}}{\mathrm{d}t} = \lambda \,\mathcal{N}(t)$$

 $\Rightarrow \mathcal{N}(t) \sim \exp(-\lambda t)$

• Resummed decay probability $\mathcal{P}(t)$

$$\mathcal{P}(t) = f(t) \mathcal{N}(t) \sim \lambda \exp(-\lambda t)$$

Parton shower branching

Differential branching probability

$$f(t) \equiv \frac{\mathcal{D}_{ij}^{(\mathrm{PS})}}{\mathcal{B}}$$

Survival probability *N*(t)

$$-\frac{\mathrm{d}\mathcal{N}}{\mathrm{d}t} = f(t)\,\mathcal{N}(t)$$

$$\Rightarrow \mathcal{N}(t) \sim \exp\left(-\int_0^t \mathrm{d}t' f(t')\right)$$

• Resummed branching probability $\mathcal{P}(t)$ $\mathcal{P}(t) = f(t) \mathcal{N}(t) \sim f(t) \exp\left(-\int_0^t dt' f(t')\right)$



Summary of main parton shower ingredients

"Sudakov form factor"
 Survival probability of parton ensemble:

$$\mathcal{N}(t) \sim \exp\left(-\int_0^t \mathrm{d}t' f(t')\right) \quad \to \quad \Delta(t',t'') = \prod_{\{ij\}} \exp\left(-\int_{t'}^{t''} \mathrm{d}t \; \frac{\mathcal{D}_{ij}^{(\mathrm{PS})}}{\mathcal{B}}\right)$$

- Evolution variable t: not time, but scale of collinearity from hard to soft t ~ 2p_ip_j ~ e.g. angle θ, virtuality Q², relative transverse momentum k²_⊥,...
- Starting scale μ_0^2 (time t = 0 in radioactive decay) defined by hard scattering
- Cutoff scale related to hadronisation scale $t_0 \sim \mu_{
 m had}^2$
- Other variables (z, ϕ) generated directly according to $d\sigma_{ii}^{(PS)}(t, z, \phi)$



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\Rightarrow Differential cross section (up to first emission)

 $d\sigma^{(B)} = d\Phi_B B$



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\Rightarrow Differential cross section (up to first emission)

$$d\sigma^{(PS)} = d\Phi_B \mathcal{B}\left[\underbrace{\Delta^{(PS)}(t_0, \mu_Q^2)}_{\text{unresolved}} + \underbrace{\sum_{\{ij\}} \int_{t_0}^{\mu_Q^2} dt \, \frac{d\sigma^{(PS)}_{ij}}{dt} \Delta^{(PS)}(t, \mu_Q^2)}_{\text{resolved}}\right]$$



$\textbf{Example: pp} \rightarrow \textbf{h+jets}$













Parton shower improvements



NLO+PS matching

- Parton shower on top of NLO prediction (e.g. inclusive W production)
- Objectives:
 - avoid double counting in real emission
 - preserve inclusive NLO accuracy

ME+PS@L0 merging

- Multiple LO+PS simulations for processes of different jet multi (e.g. W, Wj, Wjj, ...)
- Objectives:
 - combine into one inclusive sample by making them exclusive
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Combination: ME+PS@NL0

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Basic idea

- "double-counting" between emission in real ME and parton shower for first emission
- ME is better than $\text{PS} \rightarrow \text{subtract}~\text{PS}$ contribution first
- but: shower unitary \rightarrow re-add "integrated" PS contribution with Born kinematics





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- "double-counting" between emission in real ME and parton shower for first emission
- ME is better than $PS \rightarrow$ subtract PS contribution first
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Subtlety: NLO already contains subtraction

$$\mathrm{d}\sigma^{(\mathrm{NLO})} = \mathrm{d}\Phi_{B} \left[\mathcal{B} + ilde{\mathcal{V}} + \sum_{\{ij\}} \mathcal{I}^{(\mathrm{S})}_{\{ij\}}
ight] + \mathrm{d}\Phi_{R} \left[\mathcal{R} - \sum_{\{ij\}} \mathcal{D}^{(\mathrm{S})}_{ij}
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Additional subtraction

• introduce additional (shower) subtraction terms $\mathcal{D}_{ii}^{(\mathrm{A})}$

$$d\sigma^{(\text{NLO sub)}} = d\Phi_B \ \bar{\mathcal{B}}^{(\text{A})} + d\Phi_R \left[\mathcal{R} - \sum_{\{ij\}} \mathcal{D}_{ij}^{(\text{A})} \right]$$

with $\bar{\mathcal{B}}^{(\text{A})} = \mathcal{B} + \tilde{\mathcal{V}} + \sum_{\{ij\}} \mathcal{I}_{(ij)}^{(\text{S})} + \sum_{\{ij\}} \int dt \left[\mathcal{D}_{ij}^{(\text{A})} - \mathcal{D}_{ij}^{(\text{S})} \right]$

- now apply PS resummation using $\mathcal{D}^{(\mathrm{A})}_{ij}$ as splitting kernels



Frixione, Webber (2002)

Master formula for NLO+PS up to first emission

$$d\sigma^{(\text{NLO+PS)}} = d\Phi_B \bar{\mathcal{B}}^{(\text{A})} \left[\underbrace{\Delta^{(\text{A})}(t_0, \mu_Q^2)}_{\text{unresolved}} + \underbrace{\sum_{\{ij\}} \int_{t_0}^{\mu_Q^2} dt \, \frac{\mathcal{D}_{ij}^{(\text{A})}}{\mathcal{B}} \Delta^{(\text{A})}(t, \mu_Q^2)}_{\text{resolved, singular}} \right] \\ + d\Phi_R \left[\underbrace{\mathcal{R} - \sum_{\{ij\}} \mathcal{D}_{ij}^{(\text{A})}}_{\text{resolved, non-singular} \equiv \mathcal{H}^{(\text{A})}} \right]$$



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- To $\mathcal{O}(\alpha_s)$ this reproduces $d\sigma^{(NLO)}$
- Exact choice of $\mathcal{D}_{ii}^{(A)}$ distinguishes MC@NLO vs. POWHEG vs. S-MC@NLO vs. . . .
- Resolved cases: Subsequent emissions can be generated by ordinary PS



Mc@NLo

Frixione, Webber (2002)

 $\mathcal{D}^{(A)} = \mathcal{D}^{(PS)} = \text{PS}$ splitting kernels

- + Shower algorithm for Born-like events easy to implement
- "Non-singular" piece $\mathcal{R} \sum_{ij} \mathcal{D}_{ij}^{(A)}$ is actually singular:
 - Collinear divergences subtracted by splitting kernels √
 - Remaining soft divergences as they appear in non-trivial processes at sub-leading N_c

Workaround: *G*-function dampens soft limit in non-singular piece ⇔ Loss of formal NLO accuracy but heuristically shown to be negligible



Höche, Krauss, Schönherr, FS (2011)

 $\mathcal{D}^{(A)} = \mathcal{D}^{(S)} = \mbox{Subtraction terms}$

- + "Non-singular" piece fully free of divergences
- Splitting kernels in shower algorithm become negative

Solution: Weighted $N_C = 3$ one-step PS based on subtraction terms













NLO+PS matching

- Parton shower on top of NLO prediction (e.g. inclusive *W* production)
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Tree-level ME+PS merging

Main idea

Catani, Krauss, Kuhn, Webber (2001)

Phase space slicing for QCD radiation in shower evolution

- Soft/collinear emissions $Q_{ij}(z,t) < Q_{cu}$
 - \Rightarrow Retained from parton shower

$$\mathcal{D}_{ij}^{(\mathrm{PS})} = \mathcal{B} \times \left[8\pi \alpha_s \; \frac{1}{2p_i p_j} \; \mathcal{K}_{ij}(p_i, p_j)
ight]$$

- Hard emissions Q_{ij}(z, t) > Q_{cut}
 - Events rejected ~> Sudakov suppression
 - Compensated by events starting from higher-order ME regularised by Q_{cut}
 - \Rightarrow Splitting kernels replaced by exact real-emission matrix elements

$$\mathcal{D}^{(\mathrm{PS})}_{ij} \rightarrow \mathcal{R}_{ij}$$

(But Sudakov form factors $\Delta^{(PS)}$ remain unchanged)

Cross section up to first emission in ME+PS

$$d\sigma = d\Phi_B \mathcal{B}\left[\underbrace{\Delta^{(PS)}(t_0, \mu_Q^2)}_{\text{unresolved}} + \sum_{\{ij\}} \int_{t_0}^{\mu_Q^2} dt \,\Delta^{(PS)}(t, \mu^2) \\ \times \left(\underbrace{\frac{\mathcal{D}_{ij}^{(PS)}}{\mathcal{B}} \Theta(Q_{\text{cut}} - Q_{ij})}_{\text{resolved}, PS \text{ domain}} + \underbrace{\frac{\mathcal{R}_{ij}}{\mathcal{B}} \Theta(Q_{ij} - Q_{\text{cut}})}_{\text{resolved}, ME \text{ domain}}\right)\right]$$



Translate ME event into shower language

Embedding existing emissions into PS evolution

- Preserve resummation features (logarithmic accuracy)
- Determine starting scales t for PS evolution
- ⇒ Shower picture of ME event needed!

Problem: ME only gives final state, no history

- Solution: Backward-clustering (running the shower reversed), similar to jet algorithm:
- 1 Select last splitting according to shower probablities
- 2 Recombine partons using inverted shower kinematics \rightarrow N-1 particles + splitting variables for one node
- **3** Reweight $\alpha_s(\mu^2) \rightarrow \alpha_s(p_\perp^2)$
- 4 Repeat 1 3 until core process $(2 \rightarrow 2)$

Truncated shower

- Shower each (external and intermediate!) line between determined scales
- "Boundary" scales: resummation scale μ²_Q and shower cut-off t₀





Example

Diphoton production at Tevatron

- Measured by CDF Phys.Rev.Lett. 110 (2013) 101801
- Isolated hard photons
- Azimuthal angle between the diphoton pair

ME+PS simulation using SHERPA

Höche, Schumann, FS (2009)

Conclusions

Shapes described very well even for this non-trivial process/observable for both:

- Hard region, e.g. $\Delta \Phi_{\gamma\gamma} \rightarrow 0$
- Soft region, e.g. $\Delta \Phi_{\gamma\gamma} \rightarrow \pi$

Scale variations high \Rightarrow NLO needed





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Concepts continued from ME+PS merging at LO

- For each event select iet multiplicity k according to its inclusive NLO cross section
- Reconstruct branching history and nodal scales $t_0 \dots t_k$
- Truncated vetoed parton shower, but with peculiarities (cf. below)

Differences for NLO merging

- For each event select type (S or III) according to absolute XS \Rightarrow Shower then runs differently
- Sevent:

 - 1 Generate MC@NLO emission at t_{k+1}

 - 2 Truncated "NLO-vetoed" shower between t_0 and t_k : First hard emission is only ignored, no event veto

 - 3 Continue with vetoed parton shower
- Ill event:

(Truncated) vetoed parton shower as in tree-level ME+PS







ME+PS@NLO prediction for combining NLO+PS samples of multiplicities n and n + 1

$$\begin{aligned} d\sigma &= d\Phi_n \ \bar{B}_n^{(A)} \left[\Delta_n^{(A)}(t_c, \mu_Q^2) + \int_{t_c}^{\mu_Q^2} d\Phi_1 \ \frac{D_n^{(A)}}{B_n} \Delta_n^{(A)}(t_{n+1}, \mu_Q^2) \Theta(Q_{cut} - Q_{n+1}) \right] \\ &+ d\Phi_{n+1} \ H_n^{(A)} \ \Delta_n^{(PS)}(t_{n+1}, \mu_Q^2) \Theta(Q_{cut} - Q_{n+1}) \\ &+ d\Phi_{n+1} \ \bar{B}_{n+1}^{(A)} \ \underbrace{\left(1 + \frac{B_{n+1}}{\bar{B}_{n+1}^{(A)}} \int_{t_{n+1}}^{\mu_Q^2} d\Phi_1 \ K_n \right)}_{MC \ counterterm \ \rightarrow \ NLO \ vetoed \ shower} \\ &\times \left[\Delta_{n+1}^{(A)}(t_c, t_{n+1}) + \int_{t_c}^{t_{n+1}} d\Phi_1 \ \frac{D_{n+1}^{(A)}}{B_{n+1}} \Delta_{n+1}^{(A)}(t_{n+2}, t_{n+1}) \right] \\ &+ d\Phi_{n+2} \ H_{n+1}^{(A)} \ \Delta_{n+1}^{(PS)}(t_{n+2}, t_{n+1}) \ \Delta_n^{(PS)}(t_{n+1}, \mu_Q^2) \Theta(Q_{n+1} - Q_{cut}) \ + \dots \end{aligned}$$











































Höche, Krauss, Maierhöfer, Pozzorini, Schönherr, FS (2014)



- Uncertainty reduction from 79% to 19% in 2-jet bin
- Important BSM search selection: high total transverse energy
 - ightarrow major reduction of theoretical uncertainties compared to tree-level merging



Practical considerations



Perturbative uncertainties

- Unknown higher-order corrections
- Estimated by scale variations $\mu_F = \mu_R = \frac{1}{2}\mu \dots 2\mu$

Non-perturbative uncertainties

- Model uncertainties in hadronisation, hadron decays, multiple parton interactions, parton shower (evolution variable, kinematics reshuffling, infrared cut-offs)
- Estimated by variation of parameters/models within tuned ranges

Matching/merging uncertainties

- Arbitrariness of $\mathcal{D}^{(A)}$ and thus of the exponent in $\Delta^{(A)}$
 - Estimated by:
 - Variations of μ_0^2 in MC@NLO
 - (Variation of $\mathcal{R}^{\tilde{r}}$ in POWHEG)
 - Reduced by merging with higher parton multiplicities
- Choice of merging cut



Scale vs. core scale

- Multi-jet matrix elements embedded into parton shower evolution
 ⇒ Extra emissions should be evaluated with same α_s(p^{ji})
- Remaining freedom: core process scales μ_R , μ_F

Global scale setting

(SCALES parameter)

- For multi-jet merged samples the METS setter has to be used to implement the above
- For simpler fixed-order or (N)LO+PS samples without merging:
 - VAR scale setter for arbitrary functions of parton level momenta
 - FASTJET scale setter to use jet momenta
 - custom definition by writing C++ code

Core process scale

(CORE_SCALE parameter)

- For use with the METS global scale setter
- Different options to define the core scale:
 - VAR core scale setter for arbitrary functions of parton level momenta
 - DEFAULT core scale setter for automatically taking into account type of core process (cf. next slide)





- Multi-jet merging based on core process + up to *n* partons
- Core process defined by user \rightarrow unambigious? \rightarrow two options to translate ME events into shower language:

"Exclusive" merging

(EXCLUSIVE_CLUSTER_MODE=1)

- Emission history identified by QCD clustering only
 ⇒ core process as defined by user
- Most straightforward way of a shower history
- If core process contains partons, e.g. in electroweak V+2-jets production: parton level cuts for "core" jets necessary
- What if the event looks more like hard QCD with softer EW attached?







- Multi-jet merging based on core process + up to *n* partons
- Core process defined by user → unambigious?
 → two options to translate ME events into shower language:

"Inclusive" merging

(EXCLUSIVE_CLUSTER_MODE=0)

- Allow EW clusterings in emission history
 ⇒ can end up with different core process
- This core process is then also used to define the core scales (e.g. factorisation scale)





- Dedicated scale/PDF variation runs expensive, unfeasible for PDF4LHC prescription
- Instead: simultaneously keep track of variations in ME by multiple event weights
- Available since Sherpa 2.2.0 for fixed-order, S-MC@NLO and ME+PS@LO simulations
- Upcoming in next release for ME+PS@NLO as well



 Closure compared to variation in dedicated runs for pp → ttW with S-Mc@NLO



 Mainly useful for expensive MEs and unweighted events



Functional form $Q_{ij}(z,t)$

ME+PS separation determined by "jet criterion" $Q_{ij}(z, t) > Q_{cut}$

- Has to identify soft/collinear divergences in MEs, like jet algorithm
- Otherwise arbitrary functional form

Cut value Q_{cut}

- If the merging prescription works well: ME region is supplemented consistently with resummation
 - \Rightarrow merging cut can be chosen arbitrarily low
- Disadvantages of very low merging cuts:
 - higher proportion of multi-parton MEs \Rightarrow CPU time increases
 - MEs less stable, integration converges more slowly

 \Rightarrow Typically compromise between physics and costs: merging cut softer than typical jet criterion in analysis (e.g. $p_{\perp}>20\,{\rm GeV})$

- Careful with extreme phase space regions (e.g. very forward jets)!
- Dynamical definition of merging cuts for special circumstances, e.g. in photon production to capture fragmentation component



Consistent PDF and α_S usage

- Sherpa uses the same PDF and corresponding α_S parametrisation everywhere: MEs, parton shower, MPI, ...
- This implies that varying the PDF also changes the parton shower and MPI behaviour
- Since recently using NNLO PDF as default
 - PDF fits sensitive to shapes, ME+PS merging captures N(N(...))LO shapes
 - Some inclusive processes benefit significantly from usage of more reliable NNLO PDF

Tuning

- Tuning is done with a given PDF, e.g. default in Sherpa 2.2 is NNPDF 3.0 NNLO
- Should one change the full tune when using different PDFs (double counting of systematic uncertainties)? (irrelevant for on-the-fly PDF variation, since that is only available for MEs)







Negative weights

- NLO-matched simulations \Rightarrow negative weight events from subtraction terms and $N_C = 3$ shower
- Fraction of negative weights can vary
 - r = few % for simple processes
 - r = 20 30% for complex ones

 \Rightarrow effective statistical uncertainty increased by factor $\frac{1}{1-2r}$

Weight distributions

- Unweighted events would ideally have weights reduced to ± 1
- There are a few additional weights which can not be removed by unweighting
 - "Overweight" events: phase space point yields ME value larger than the maximum found during integration
 - $N_C = 3$ shower weights
 - "local K-factor" for LO multiplicities on top of NLO
 - \Rightarrow (steeply falling) weight distribution around ± 1



- Experiment software prefers tree-like event records with straightened mother-daughter relations
- This is not necessarily the case in Sherpa:



- Dipole-like parton showers imply there is no distinction between ISR and FSR ⇒ Parton shower "blob" can lead to particle "loops"
- (New option in Sherpa 2.2 removes the inside of shower blobs to give straight event record)



Conclusions



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- Objectives:
 - combine into one inclusive sample
 - preserve NLO accuracy for jet observables



Outlook

- Skipped today: NNLO+PS matching in Sherpa Höche, Li, Prestel (2014)
- ⇒ Perturbative accuracy covered with new approaches in recent years
 - Big effort on bringing the improvements into full production within experiments
 - Experimental validation
 - Feasibility for (unweighted) event generation with highest accuracies
 - User support for new practical issues
 - Future focus on improvement of resummation accuracy in parton showers



Backup



Original POWHEG

Choose additional subtraction terms as

$$\mathcal{D}_{ij}^{(\mathrm{A})} o
ho_{ij} \mathcal{R} \quad \text{where} \quad
ho_{ij} = rac{\mathcal{D}_{ij}^{(\mathrm{S})}}{\sum_{nm} \mathcal{D}_{nn}^{(\mathrm{S})}}$$

- \mathcal{H} -term vanishes \Rightarrow No negative weighted events
- Similar to PS with ME-correction for 1st emission (e.g. Herwig, Pythia)

Mixed scheme

• Subtract arbitrary regular piece from $\mathcal R$ and generate separately as $\mathbb H$ -events

$$\mathcal{D}_{ij}^{(A)}(\Phi_R) \to \rho_{ij}(\Phi_R) \left[\mathcal{R}(\Phi_R) - \mathcal{R}^r(\Phi_R) \right] \quad \text{where} \quad \rho_{ij} \text{ as above}$$

- Tuning of \mathcal{R}^r to reduce exponentiation of arbitrary terms
- Allows to generate the non-singular cases of ${\mathcal R}$ without underlying ${\mathcal B}$