

# Monte Carlo Tools

[ Aspen 2012 Winter Conference ]

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Jan Winter <sup>a</sup>

– CERN –

→ *Try to cover ...*

- *recent developments ...  
... by talking about selected topics.*
- *Focus is on how to combine MEs and PSs ...*
- *... in various ways.*

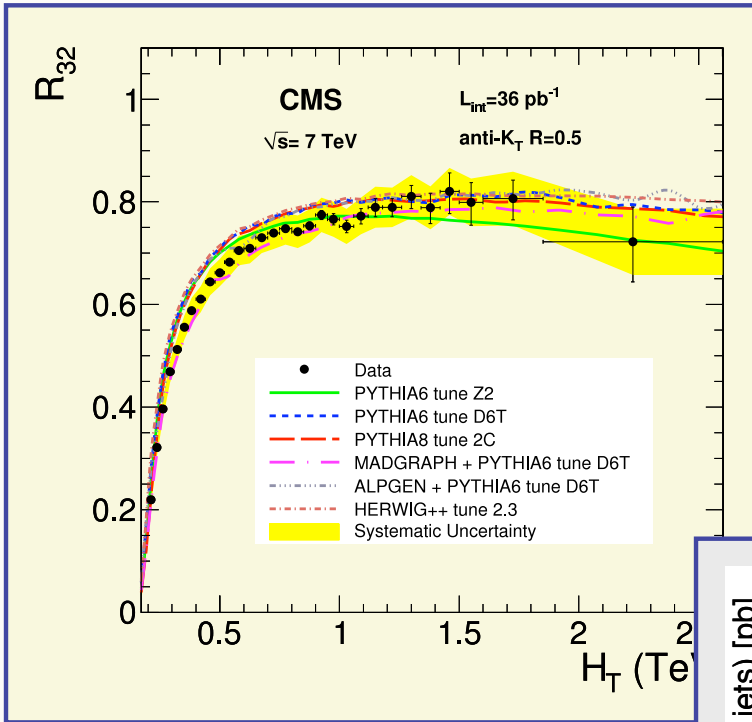
<http://www.sherpa-mc.de/>

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<sup>a</sup>Sherpa authors: S. Höche, H. Hoeth, F. Krauss, M. Schönherr, F. Siegert, S. Schumann, J. Winter and K. Zapp



# Monte Carlo tools at work



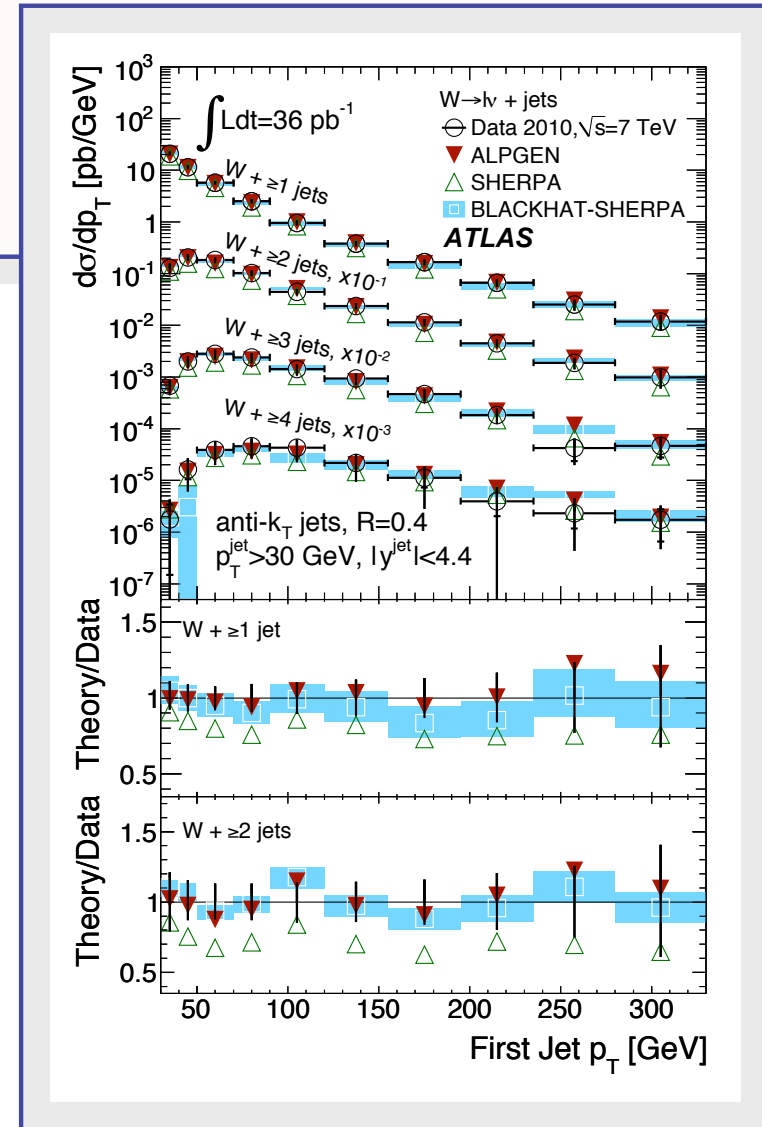
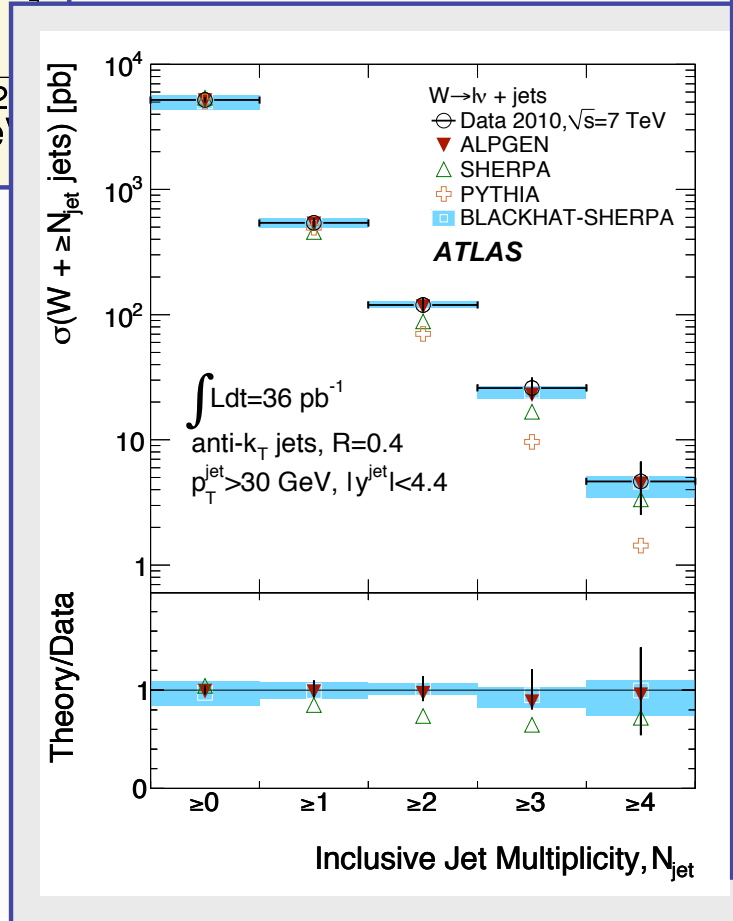
ATLAS:  $W + \text{jets}$  with 36/pb

[ARXIV:1201.1276]

**CMS:** Ratio of 3-jet to 2-jet xsec as function of  $H_T$

[ARXIV:1106.0647]

various Monte Carlo predictions compared to data.



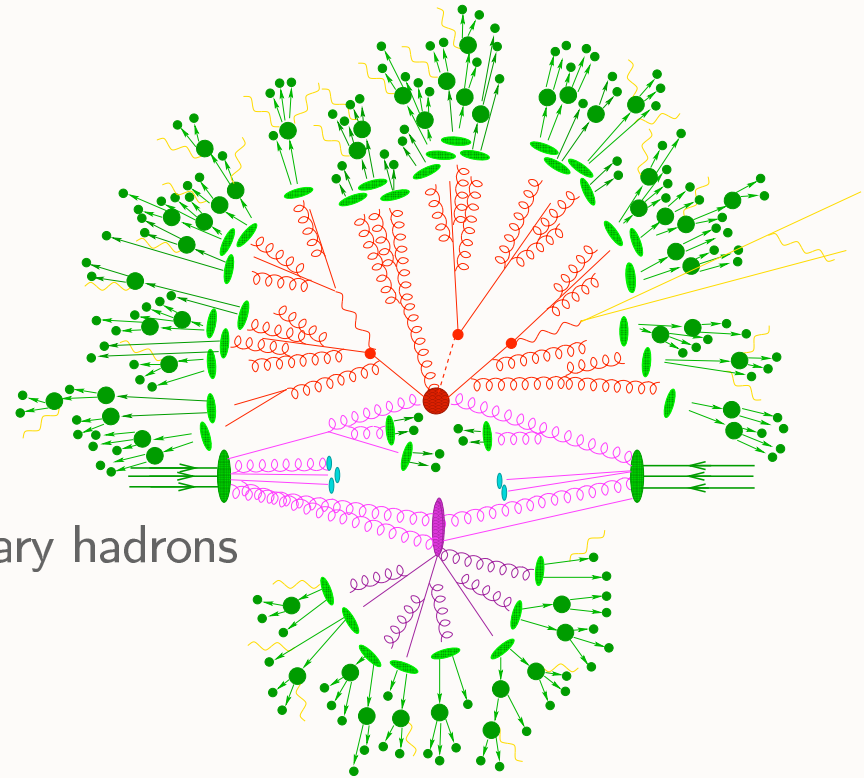
# Monte Carlo event generation

*Event generators used to model the **multi-hadron** final states of high-energy particle collisions.  
Factorization approach: divide jet simulation into different phases – use Monte Carlo methods.*

- ➔ *Perturbative Phases: [parton jets]*
- *Hard process/interaction (hard jet production)*  
exact matrix elements  $|\mathcal{M}|^2$
- *QCD bremsstrahlung (soft/coll multiple emissions)*  
initial- and final-state parton showering
- *Multiple/Secondary interactions*  
modelling the underlying event
- ➔ *Non-perturbative Phases: [jet confinement – particle jets]*

- *Hadronization*  
phenomenological models to convert partons into primary hadrons
- *Hadron decays*  
phase-space or effective models to decay unstable into stable hadrons as observed in detectors

➔ predictions at hadron level – comparable to experimental data if corrected for detector effects

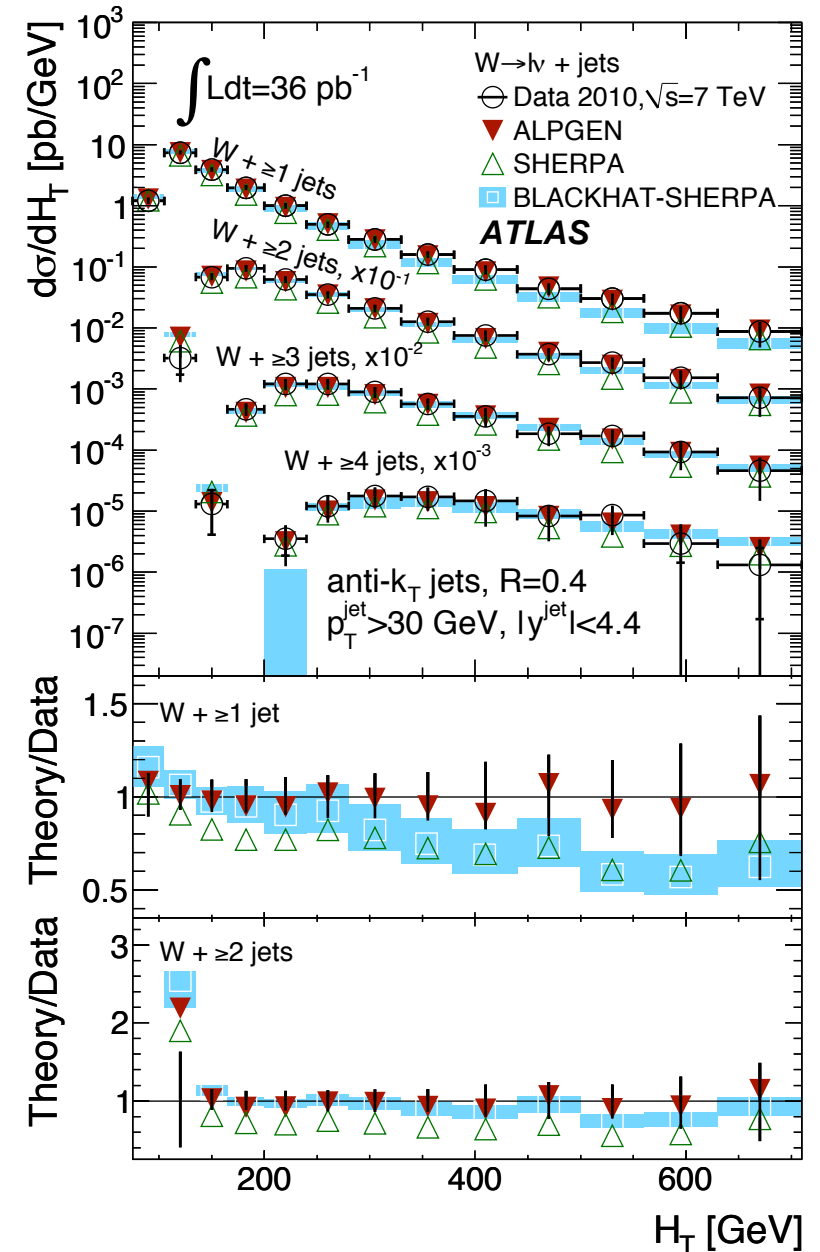
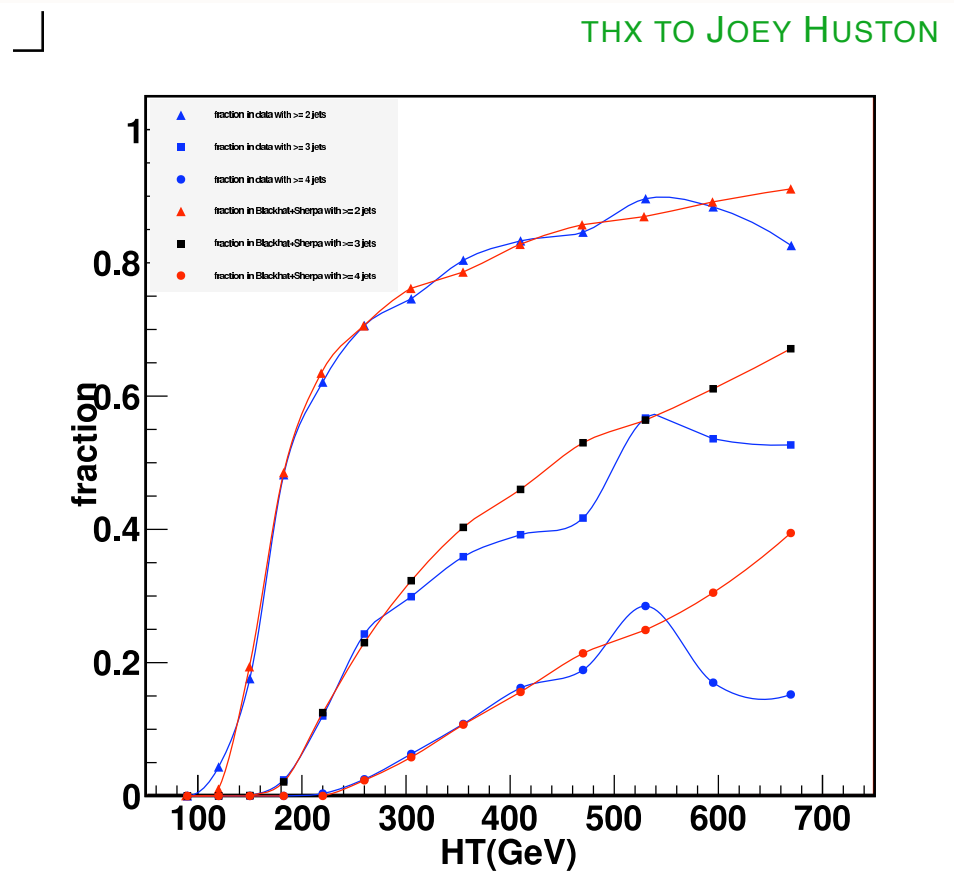


# HT distribution in recent ATLAS measurement

[ATLAS COLLABORATION (GEORGES AAD ET AL.), ARXIV:1201.1276 [HEP-EX]]

➔ *HT ... scalar pT sum of jets, lepton and MET,*

- in different inclusive  $W + n$ -jet bins.
- particularly problematic, large  $H_T$  area for  $W + 1$ -jet.
- below, inclusive xsec ratios as function of  $H_T$ .



# HT distribution in recent ATLAS measurement

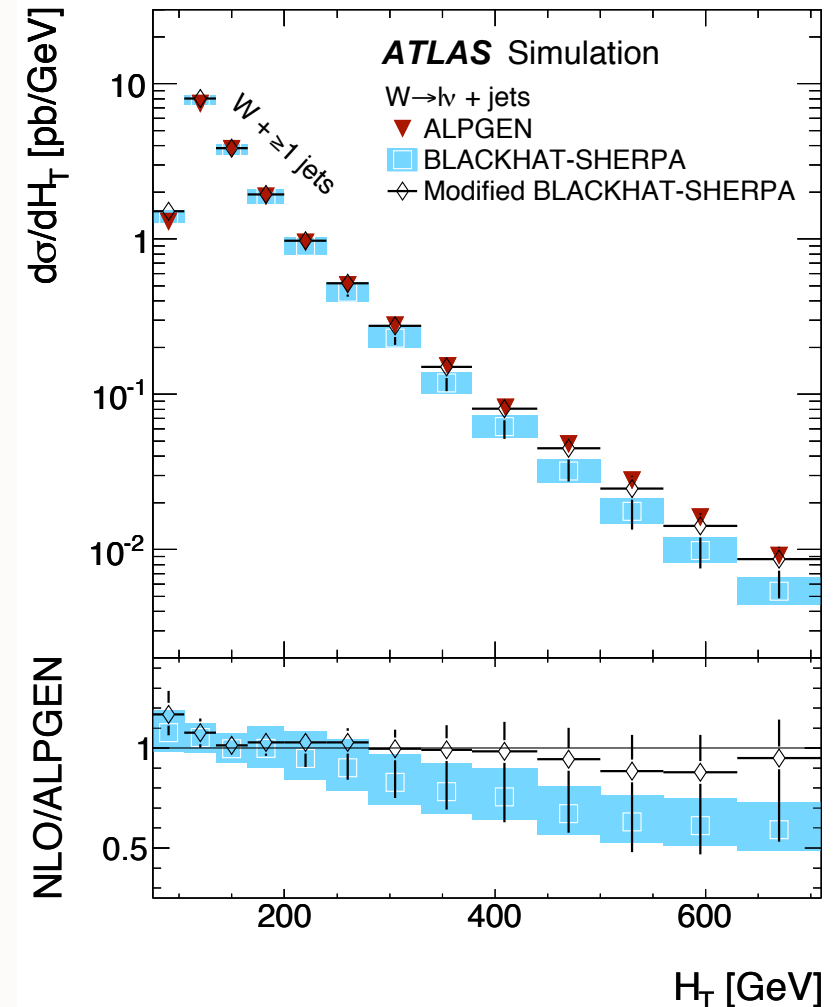
[ATLAS COLLABORATION (GEORGES AAD ET AL.), ARXIV:1201.1276 [HEP-EX]]

➔ *HT ... scalar pT sum of jets, lepton and MET in inclusive W+1-jet bin.*

- Alpgen gives fantastic agreement, use as reference.
- Sherpa's problem here: default scale & PDF choices not optimal.
- BlackHat+Sherpa's problem:  $W + 1$ -jet NLO calculation is not valid in this high  $H_T$  region.

- Modified BlackHat+Sherpa is attempt to combine various  $W + n$ -jet NLO calculations ( $n = 1, \dots, 4$ ) avoiding double counting of contributions:
  - ➔  $n$ -jet prediction only describes  $n$ -jet events
  - ➔  $n + 1$ -jets allowed for highest multiplicity

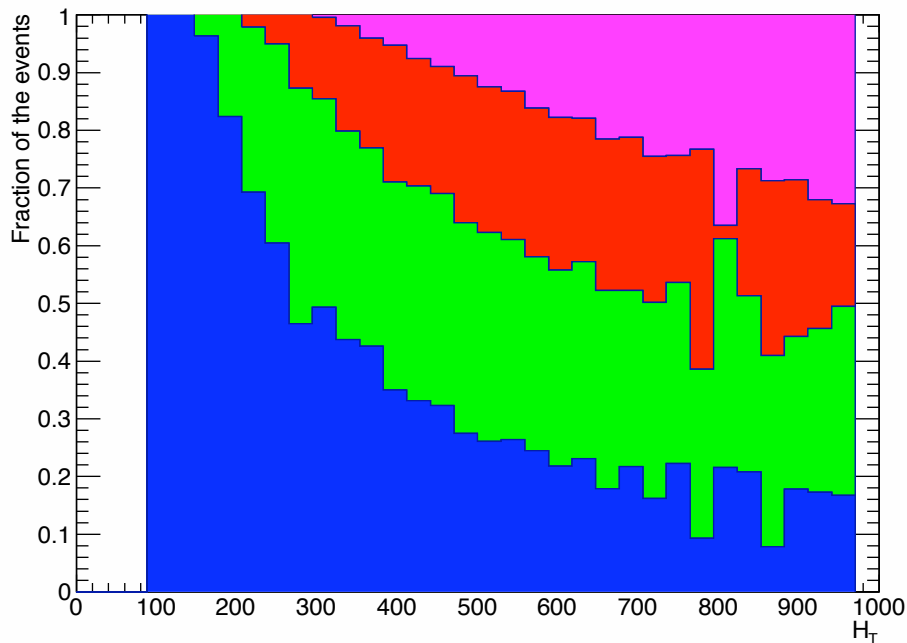
$$\sigma^{\text{tot}} \equiv \sigma_m^{\text{inc}} = \sum_{n=m}^{M-1} \sigma_n^{\text{exc}} + \sigma_M^{\text{inc}} .$$



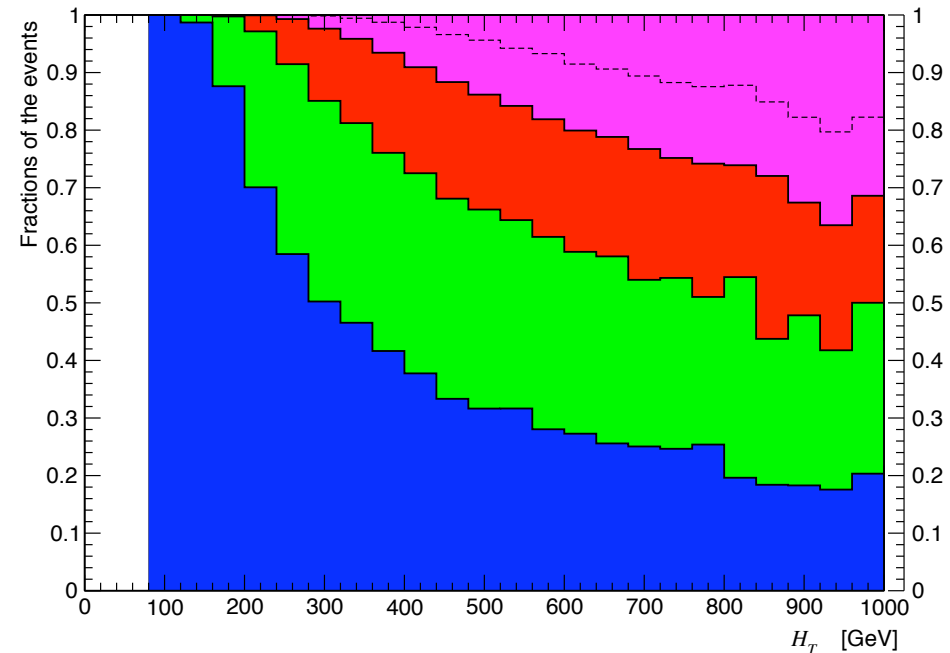
# W production in association with at least 2 jets

[ANDERSEN, MAÎTRE, SMILLIE, WINTER; LES HOUCHES 2011 PROCEEDINGS]

- studying the significance of multi-jet contributions in description of various observables
- colour code:  $W + 2, 3, 4, 5$  jets, last bin inclusive;  $\langle N \rangle = (\sum_{2,3,4}^i n_i^{\text{exc}} + 5 n_5^{\text{inc}}) / n_2^{\text{inc}}$
- relative multiplicity fractions and average number of jets  $\langle N \rangle$  as functions of  $H_T$  and  $H_{T,2}$
- fraction of  $W + \geq 4$  jets as large as 50% for large  $H_T$ , amplified in  $\langle N \rangle(H_T)$
- composition of inclusive  $W + 2$  jet predictions remarkably similar in all cases



BlackHat+Sherpa NLO exclusive sums

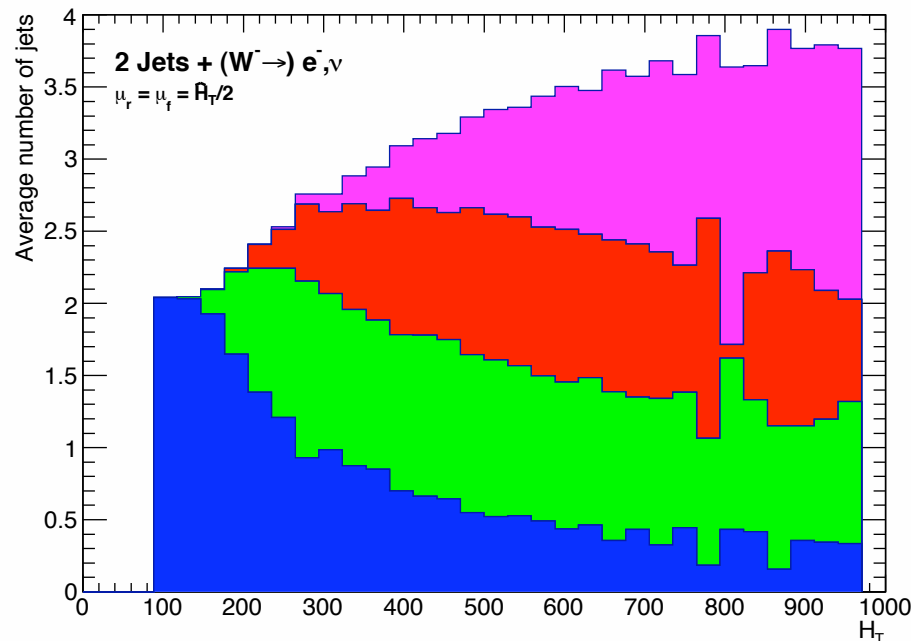


Sherpa ME+PS merging up to 5 jets

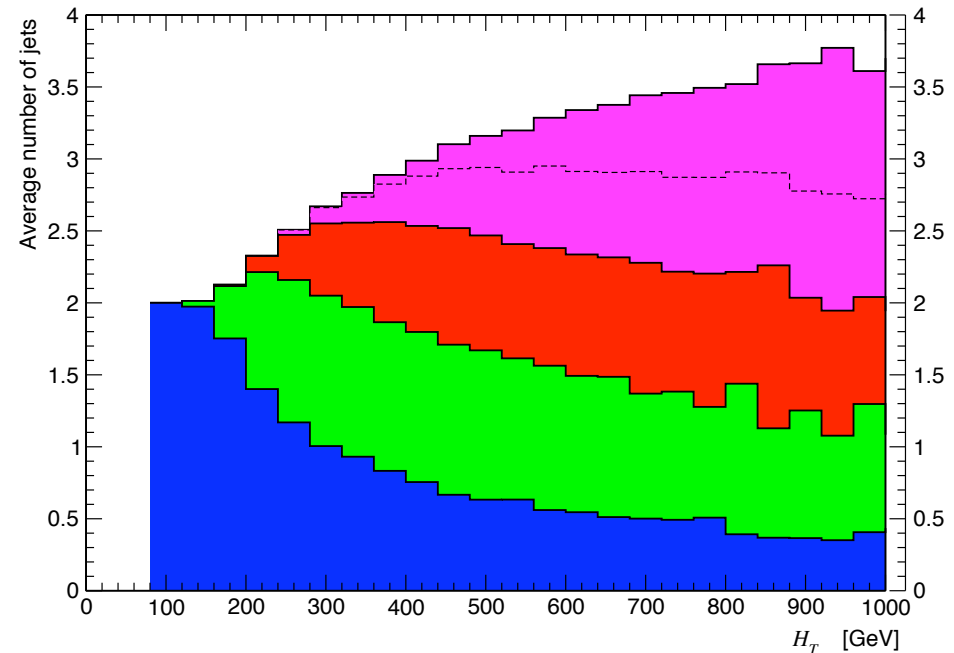
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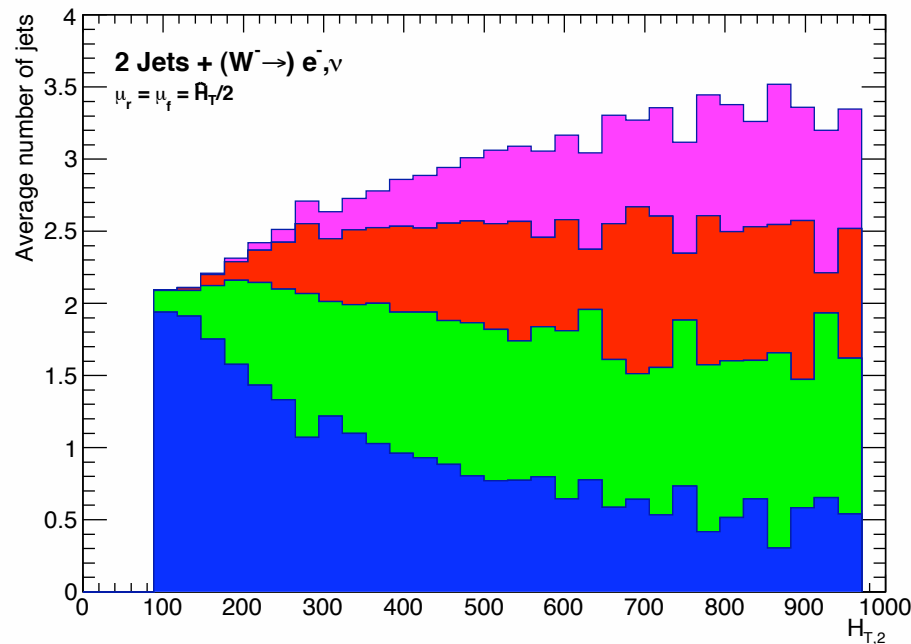


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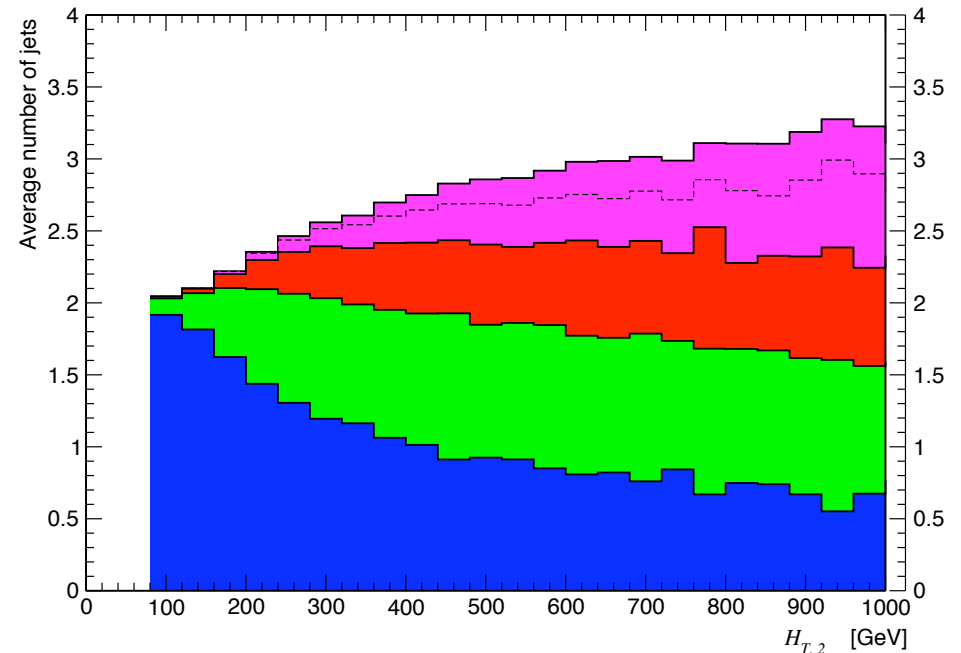
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BlackHat+Sherpa NLO exclusive sums



Sherpa ME+PS merging up to 5 jets



# (Automated) Matrix-elements frontier

[SLIDE FROM STEFAN HÖCHE]

## Cutting edge: Automating multi-leg NLO calculations

$$d\sigma^{NLO} = d\Phi_B (B + V) + d\Phi_R R = d\Phi_B [(B + V + I) + d\Phi_{R|B} (R - S)]$$

$S$  - subtraction term constructed such that IR singularities in  $R$  are removed

$I$  - integrated subtraction term locally compensates  $S \rightarrow 0 \stackrel{!}{=} I - \int d\Phi_{(1)} S$

$S$  and  $I$  universal and “easy” to automate,  $V$  tedious

⇒ Two pieces combined using the Binoth Les Houches accord CPC181(2010)1612

- One-Loop-Engine → virtual piece  
BlackHat, GOLEM, HELAC, MADLOOP, MCFM, NLOJET++, Rocket, Samurai, ...
- MC → Born, real emission, subtraction and phase space  
SHERPA, HELAC, MADDIPOLE, MADFKS, ...

Example:  $W+4$  jets with BlackHat [Berger et al.] PRL 106(2011)092001

no. jets	$W^-$ LO	$W^-$ NLO	$W^+/W^-$ LO	$W^+/W^-$ NLO	$W^-_{n/(n-1)}$ LO	$W^-_{n/(n-1)}$ NLO
0	1614.0(0.5) <sup>+208.5</sup> <sub>-235.2</sub>	2077(2) <sup>+40</sup> <sub>-31</sub>	1.656(0.001)	1.580(0.004)	—	—
1	264.4(0.2) <sup>+22.6</sup> <sub>-21.4</sub>	331(1) <sup>+15</sup> <sub>-12</sub>	1.507(0.002)	1.498(0.009)	0.1638(0.0001) <sup>+0.044</sup> <sub>-0.031</sub>	0.159(0.001)
2	73.14(0.09) <sup>+20.81</sup> <sub>-14.92</sub>	78.1(0.5) <sup>+1.5</sup> <sub>-4.1</sub>	1.596(0.003)	1.57(0.02)	0.2766(0.0004) <sup>+0.051</sup> <sub>-0.037</sub>	0.236(0.002)
3	17.22(0.03) <sup>+8.07</sup> <sub>-4.95</sub>	16.9(0.1) <sup>+0.2</sup> <sub>-1.3</sub>	1.694(0.005)	1.66(0.02)	0.2354(0.0005) <sup>+0.034</sup> <sub>-0.025</sub>	0.216(0.002)
4	3.81(0.01) <sup>+2.44</sup> <sub>-1.34</sub>	3.55(0.04) <sup>+0.08</sup> <sub>-0.30</sub>	1.812(0.001)	1.73(0.03)	0.2212(0.0004) <sup>+0.026</sup> <sub>-0.020</sub>	0.210(0.003)

# Multi-jet predictions @ LO+LL and beyond

**Traditional approach: parton showers describe additional jet activity. There are limitations:**

- semi-classical picture; quantum interferences and correlations only approximate
- lack of high-energetic large-angle emissions (LO+LL)
- shower seeds are (QCD) LO processes only, and evolution proceeds in large  $N_C$  limit
- uncertainties hard to assess & not so small; compensate for missing PT by non-PT tuning?

**Possible improvements:**

- first few hardest emissions given by tree-level MEs → improved LO+LL predictions  
[ called (tree-level/LO) ME+PS merging – CKKW, CKKW-L, MLM, ME&TS – No NLO xsecs! ]
- use NLO QCD core processes and match to parton showers → NLO+LL predictions  
[ called NLO+PS matching – MC@NLO, POWHEG – Full NLO xsecs! ]
- MENLOPS → originally combination of POWHEG and ME+PS  
[ nowadays, core: NLO+PS & additional multiplicities: ME+PS ]

**Systematic embedding of higher-order QCD corrections in multi-purpose Monte Carlos like Herwig, Pythia or Sherpa.** (enormous progress in last 10 years with two effects)

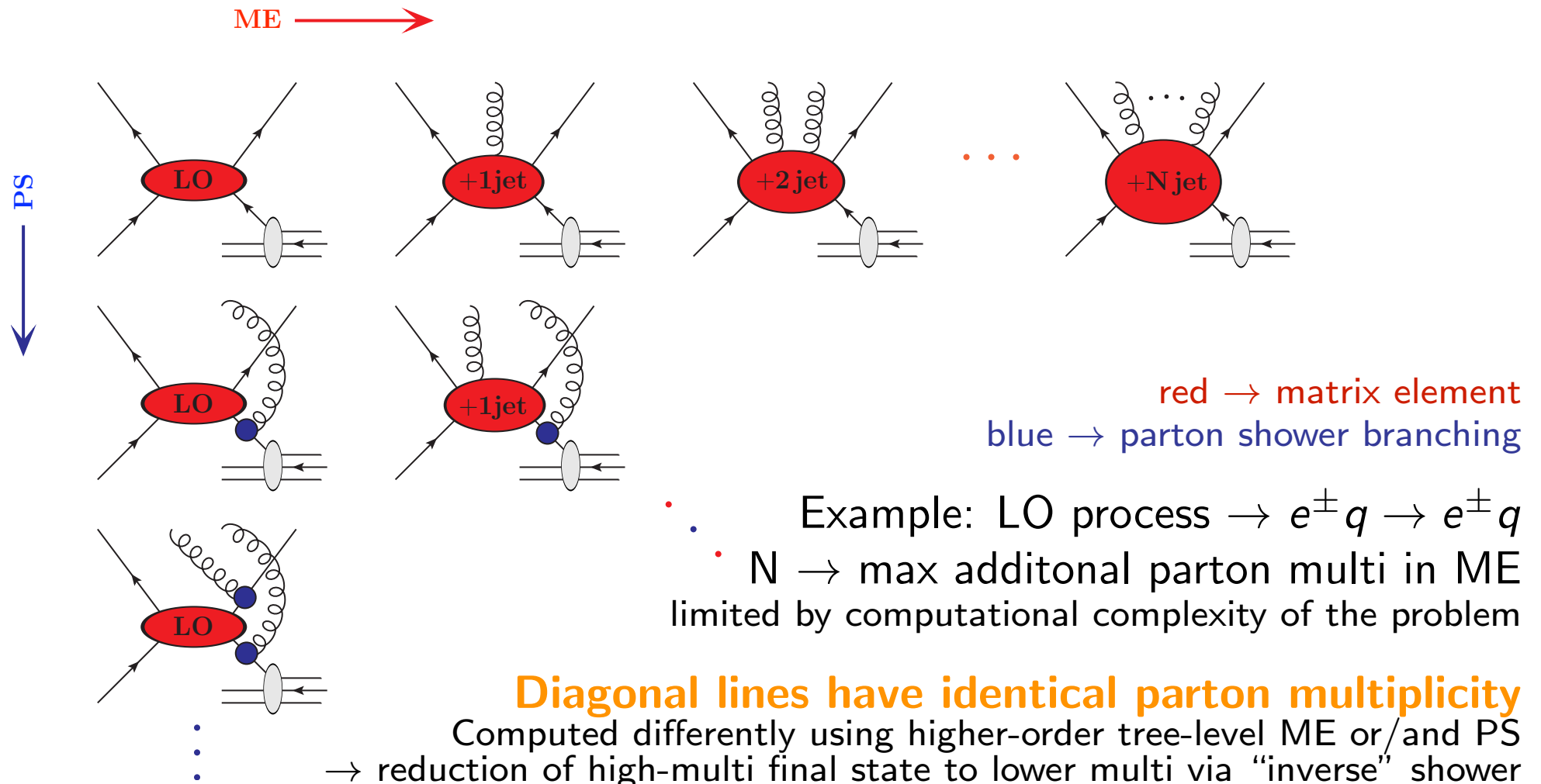
- ⇒ qualitatively better description of QCD jet data at all colliders (LEP, Hera, Tevatron, LHC)
- ⇒ improved handling and understanding of systematic uncertainties

# (LO) Matrix-element + parton-shower merging

→ combine PS pros (resumming soft emissions) + ME pros (hard emissions, quantum interferences, correlations)

⇒ Fully populate emission's phase space with either ME or PS – avoid dead regions.

⇒ ME and PS describe the same final state – remove double counting.



# Tree-level ME+PS merging

*Merging procedures have main steps in common:*

- (1) calculate  $n$ -jet cross sections: use jet criteria to define/regularize the MEs,
- (2) generate hard-parton samples with ME kinematics and  $P \propto n$ -jet/total xsecs,
- (3) accept/reject jet configurations based on their (further) PS evolution,
- (4) find suitable starting conditions for the parton showering and veto unwanted jets.

Different methods use different techniques in dealing with (1), (3) and (4):

- **CKKW**, for example: (1) employ  $k_T$ -jet measure; (3) reweight MEs through  $\alpha_s$  and analytical Sudakov form factors; (4) evolve each ME parton using  $k_T$  cluster scales & veto emissions above  $Q_{\text{jet}}$

*Examples for ME+PS merging Monte Carlos:*

- Alpgen – MLM; interfaced to Pythia or Herwig [MANGANO ET AL.]
  - MadGraph – MLM, cone or  $k_T$  jets; interfaced to Pythia [MALTONI ET AL.]
  - Sherpa – CKKW, ME&TS from vs1.2; truly interconnected with PSs [KRAUSS ET AL.]
  - Herwig++ – modified CKKW, i.e. truncated showers [RICHARDSON ET AL.]
  - Ariadne/Pythia8 – CKKW-L; combination with interleaved showers [LÖNNBLAD ET AL.]
- By and large predictions agree [HEP-PH/0602031, EPJC53(2008)473, PHYS.REPT.504(2011)145]

# Tree-level ME+PS merging

Merging

- (1) calculate  $n$ -jet cross sections
- (2) generate hard-parton events
- (3) accept/reject jet configurations
- (4) find suitable starting scales

Different methods use different

● **CKKW**, for example:  
through  $\alpha_s$  and analytical resummation  
using  $k_T$  cluster scales & K-factor

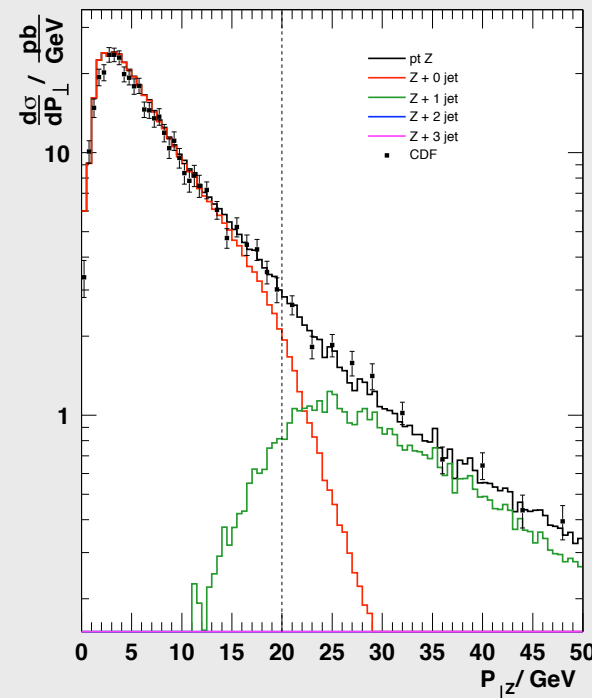
- Alpgen – MLM
- MadGraph – CKKW
- Sherpa – CKKW
- Herwig++ – CKKW
- Ariadne/Pythia – CKKW

● By and large predictions

## CKKW

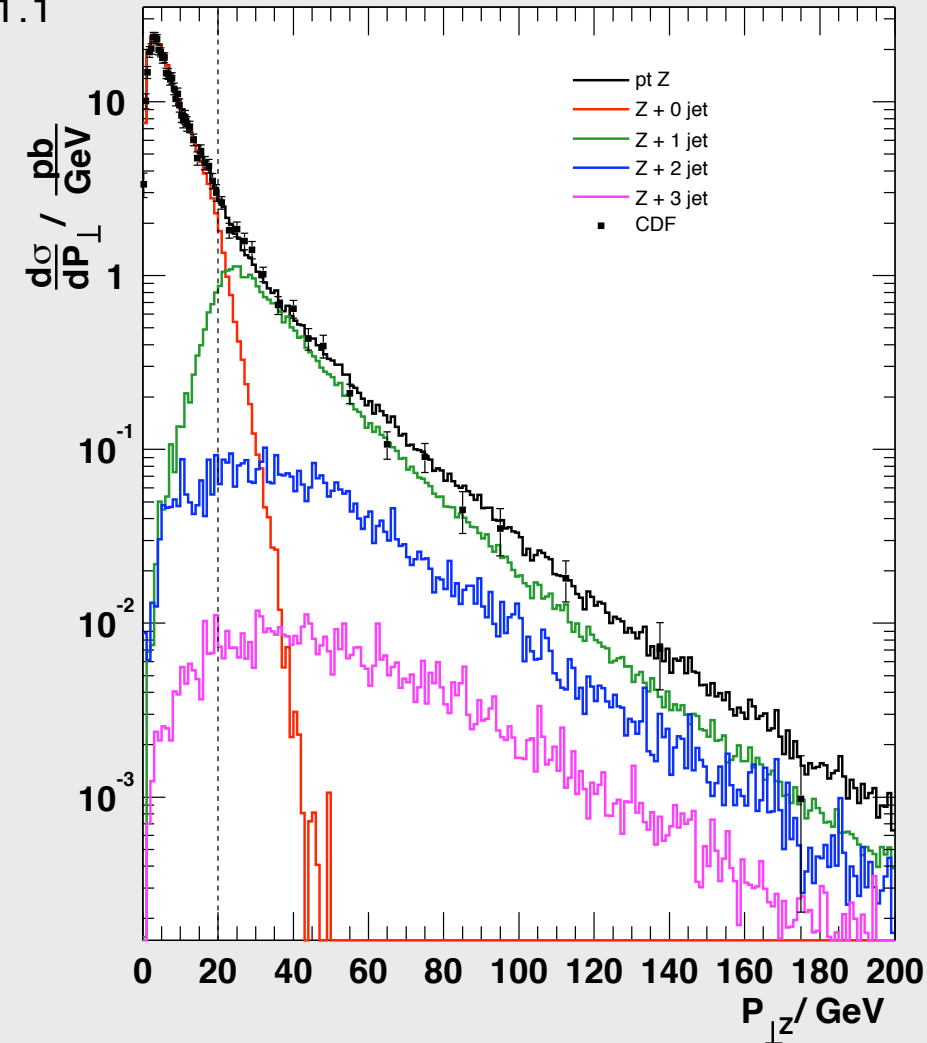
⇒ IN SHERPA VS1.0 AND VS1.1  
E.G. Z + JETS @ 1.8 TEV

- AMEGIC + APACIC
- constant K-factor
- intrinsic  $k_T$ -smearing of order 1 GeV



[CATANI, KRAUSS, KUHN, WEBBER, JHEP 11 (2001) 063]

[KRAUSS, JHEP 08 (2002) 015]



KRAUSS ET AL. PRD 70 (2004) 114009

# Systematic uncertainties of ME+PS predictions

## → *related to ME+PS merging*

- $Q_{\text{cut}}$  – magnitude of phase-space separation cut [cancels to log-accuracy of shower]
- $N_{\text{ME}}^{\text{max}}$  – maximum number of jets from hard tree-level MEs
- [ choice of internal jet separation measure ]

## → *related to pQCD :: dynamical and local scale choices*

- scale uncertainties from MEs [renormalization and factorization scale settings]
- scale uncertainties from PSs [coupling and PDF scale settings]

## → *related to pQCD–npQCD transition*

- parton-shower IR cut-off / intrinsic transverse momentum [tuned @ LEP & low- $p_T$  DY pair production]
- PDFs plus  $\alpha_s(M_Z)$  taken from the fit [enter globally, affect ME and PS]

## → *related to npQCD* [phenomenological universal models need be tuned to data]

- hadronization parameters [PROFESSOR tune against LEP data]
- underlying event parameters [PROFESSOR tune mainly against LHC data]

Les Houches 2011:

Step-by-step systematics study.

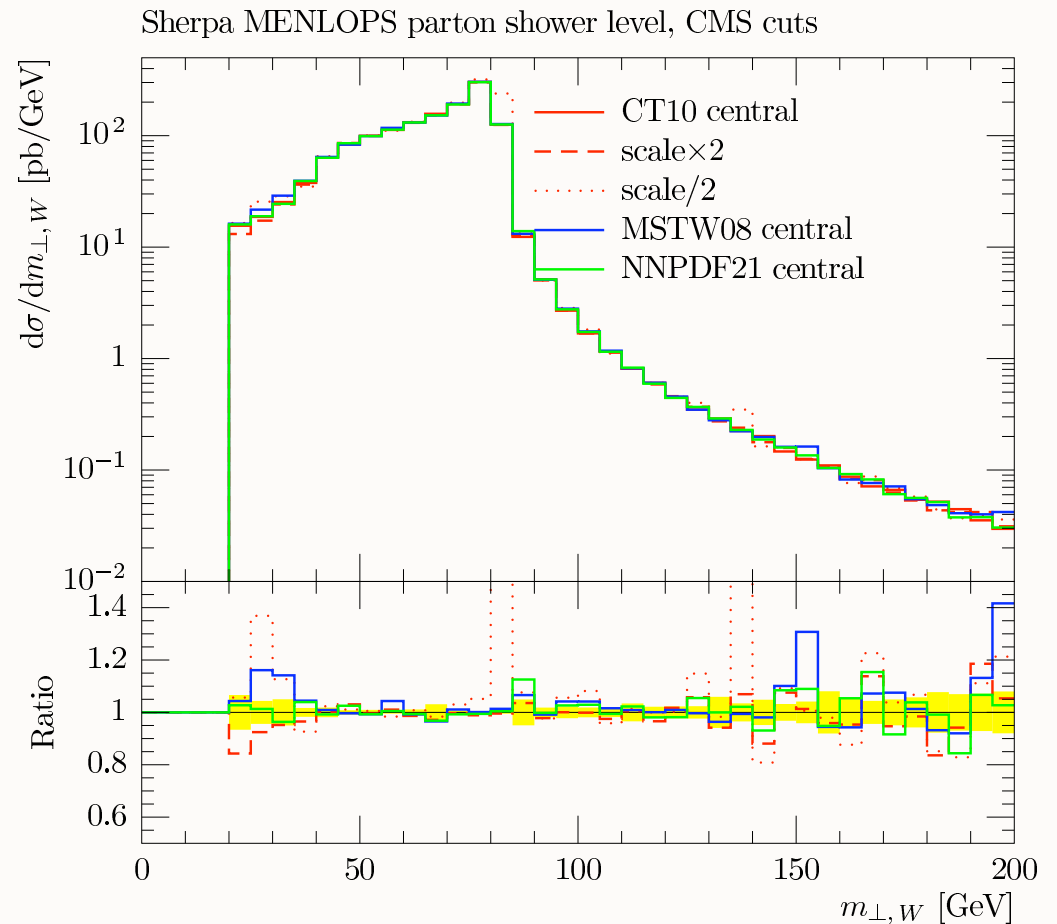
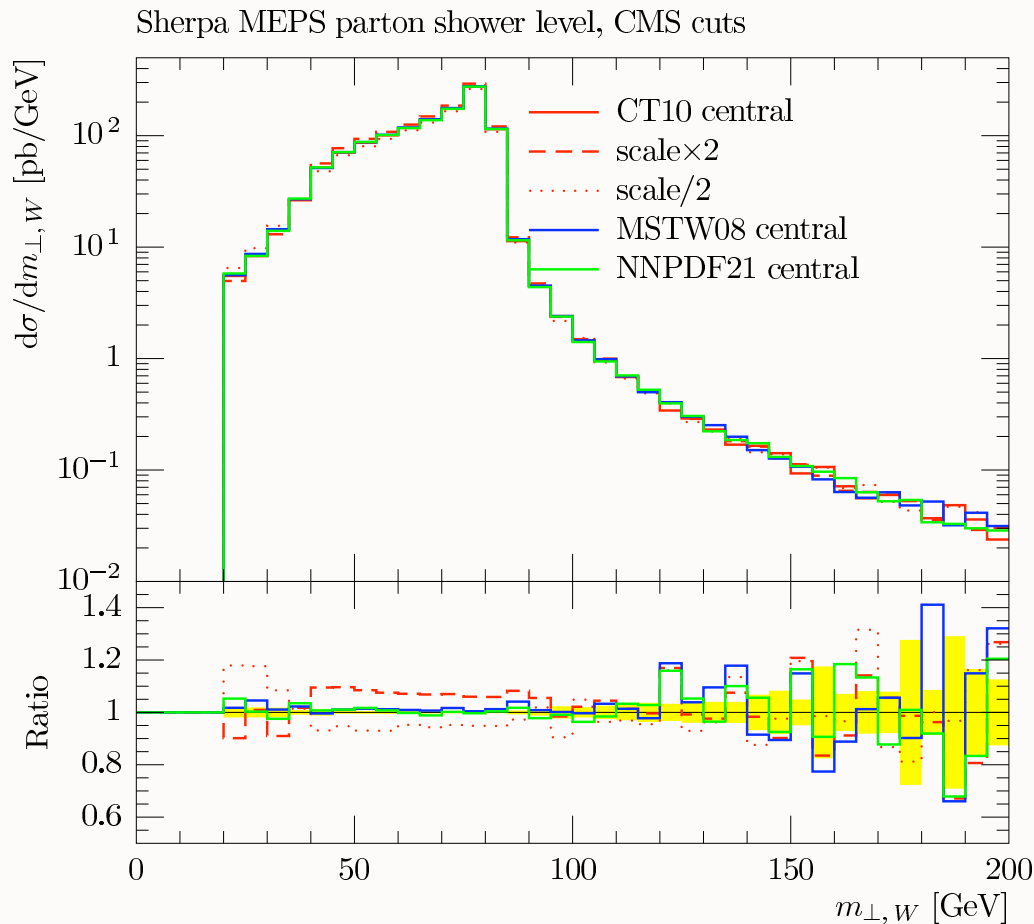
Estimate and understand uncertainties related to each source.

# Step-by-step systematics study

[ALIOLI ET AL. LES HOUCHEs 2011 PROCEEDINGS]

## ➔ Example: transverse mass of $W$ boson in Sherpa using $ME+PS$ and $MENLOPS$ .

- factorization and renormalization scale variations affecting ME and PS domain
- MENLOPS has smaller scale uncertainties due to NLO accuracy of core process
- PDF uncertainties estimated by comparing different PDF sets

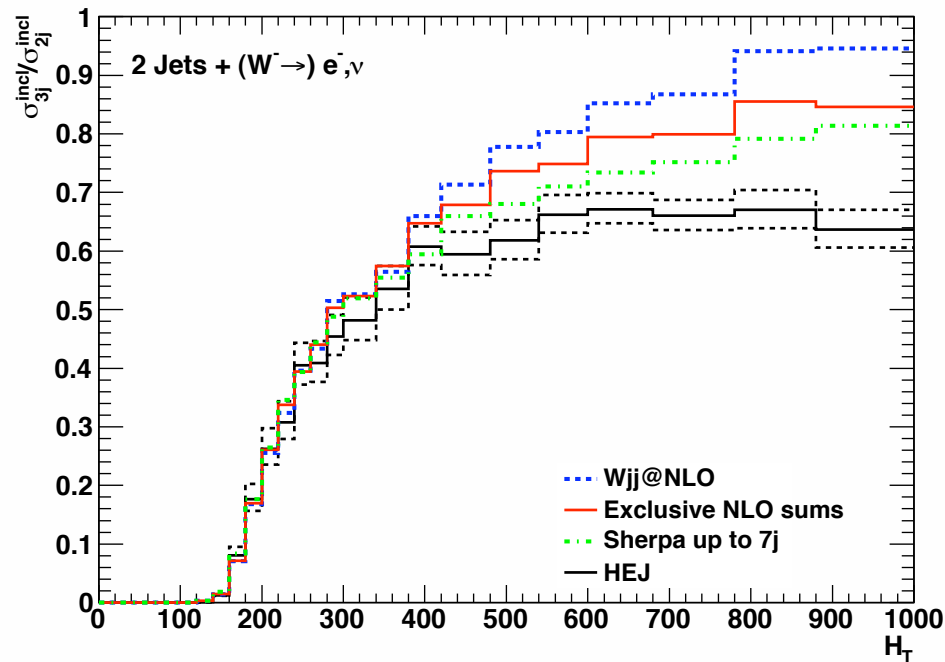
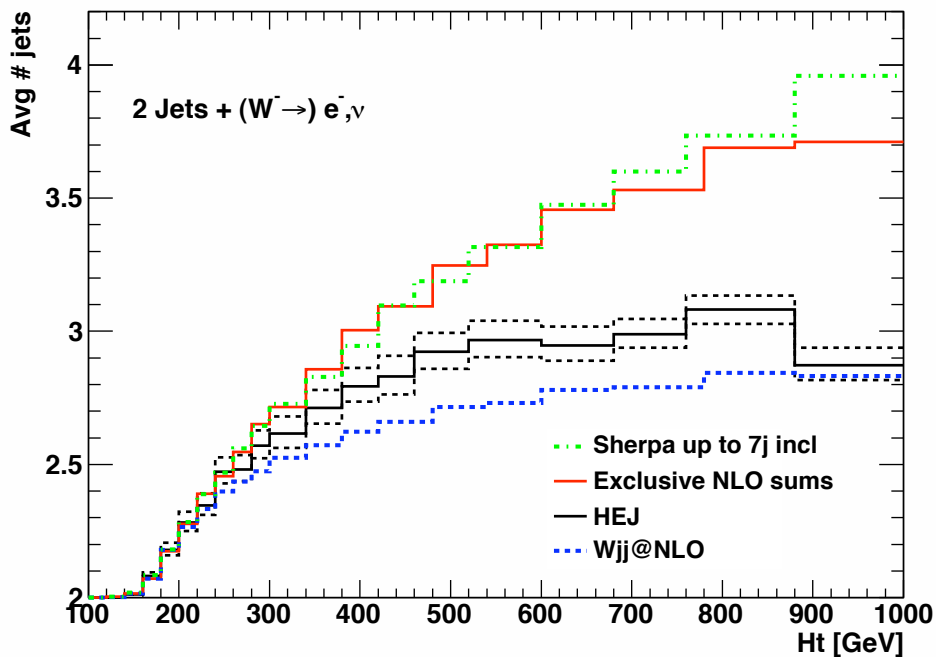


# Once more, $W$ bosons in association with at least 2 jets

[ANDERSEN, MAÎTRE, SMILLIE, WINTER; LES HOUCHES 2011 PROCEEDINGS]

## → Average number of jets and ratio of 3-jet to 2-jet rate as a function of $H_T$ .

- including the predictions of HEJ (High Energy Jets, an all-order resummation of wide-angle radiation) [ANDERSEN, SMILLIE]
- and of the  $W + 2$  jets BlackHat+Sherpa calculation.
- More data will allow to discriminate the approaches.
- Again, NLO exclusive sums and Sherpa ME+PS look rather similar.





# NLO exclusive sums versus ME+PS

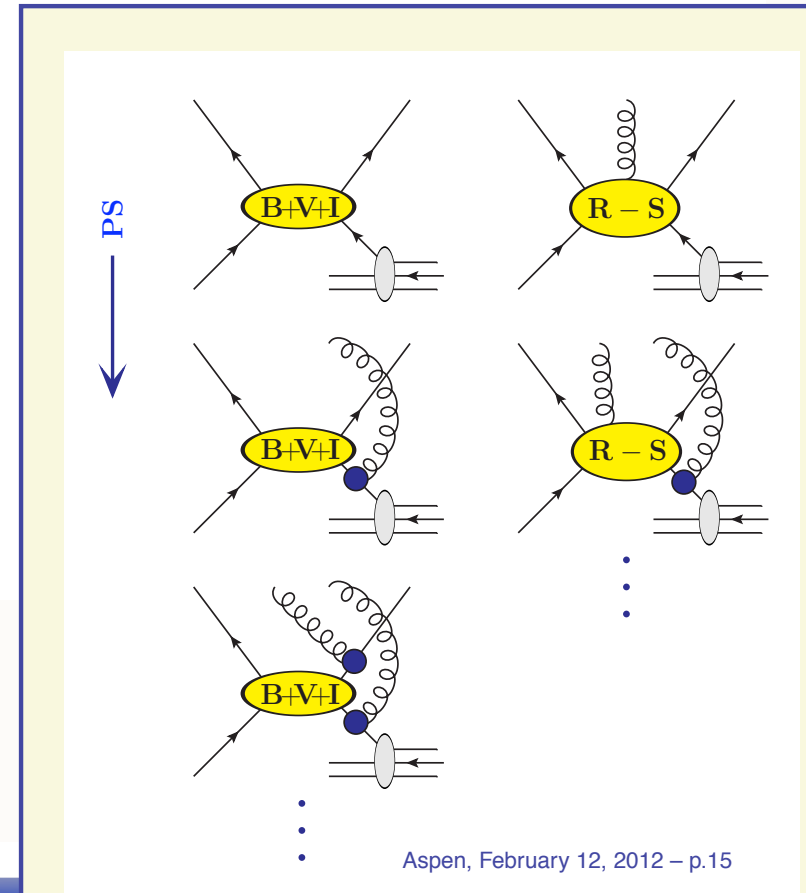
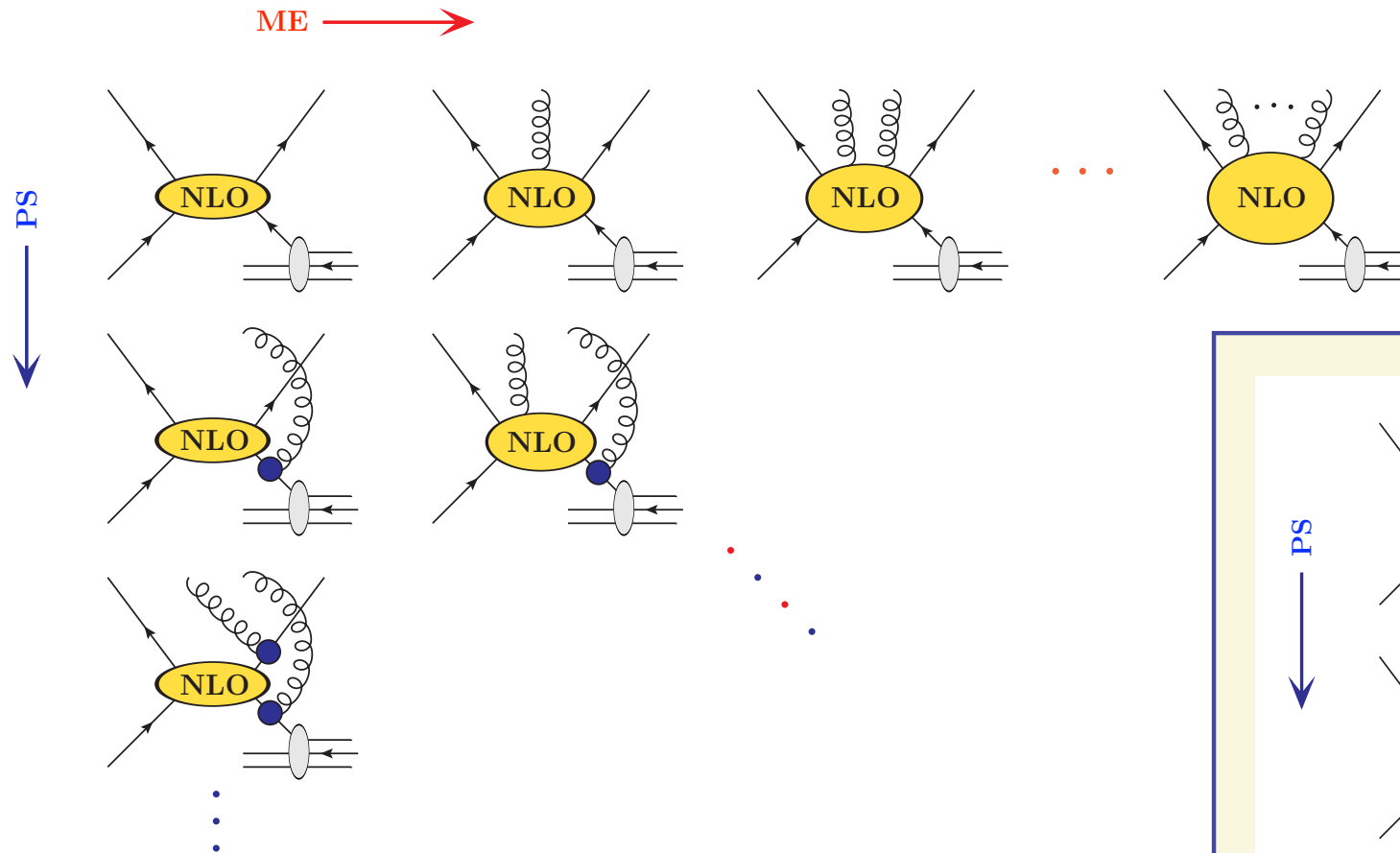
➔ *Decompose total cross section based on exclusive and inclusive jet bins.*

$$\sigma^{\text{tot}} \equiv \sigma_m^{\text{inc}} = \sum_{n=m}^{M-1} \sigma_n^{\text{exc}} + \sigma_M^{\text{inc}}$$

- NLO exclusive sums: each jet bin at NLO accuracy, i.e.  $\mathcal{O}(\alpha_s^{n+1})$
- terms are hence summed at different orders of  $\alpha_s$  and there is no detailed treatment of jet vetoing  
⇒ exclusive sums introduce artefacts
- for example, scale dependence of exclusive sums is not under good control
- ME+PS: each jet bin at least at LL (soft/collinear) accuracy improved by LO  $n$ -jet effects
- terms are summed at the same (infinite) order of  $\alpha_s$  and jet vetoing is LL accurate  
⇒ Similarity likely due to inclusion of same set of tree-level MEs and unresolved  $\mathcal{O}(\alpha_s)$  corrections (encoded in Sudakov form factors)  
⇒ ME+PS is LO exclusive sums combined at LL accuracy
- Way to go: bring all terms in NLO exclusive sum to same order of strong coupling  
⇒ include (approx.)  $x$ -loop corrections to all terms but highest, e.g. by using LoopSim [RUBIN, SALAM, SAPETA, JHEP1009(2010)084]  
⇒ do ME+PS trick at NLO ➔ **construction zone**

# Future goal

## ME+PS merging with multiple NLO processes



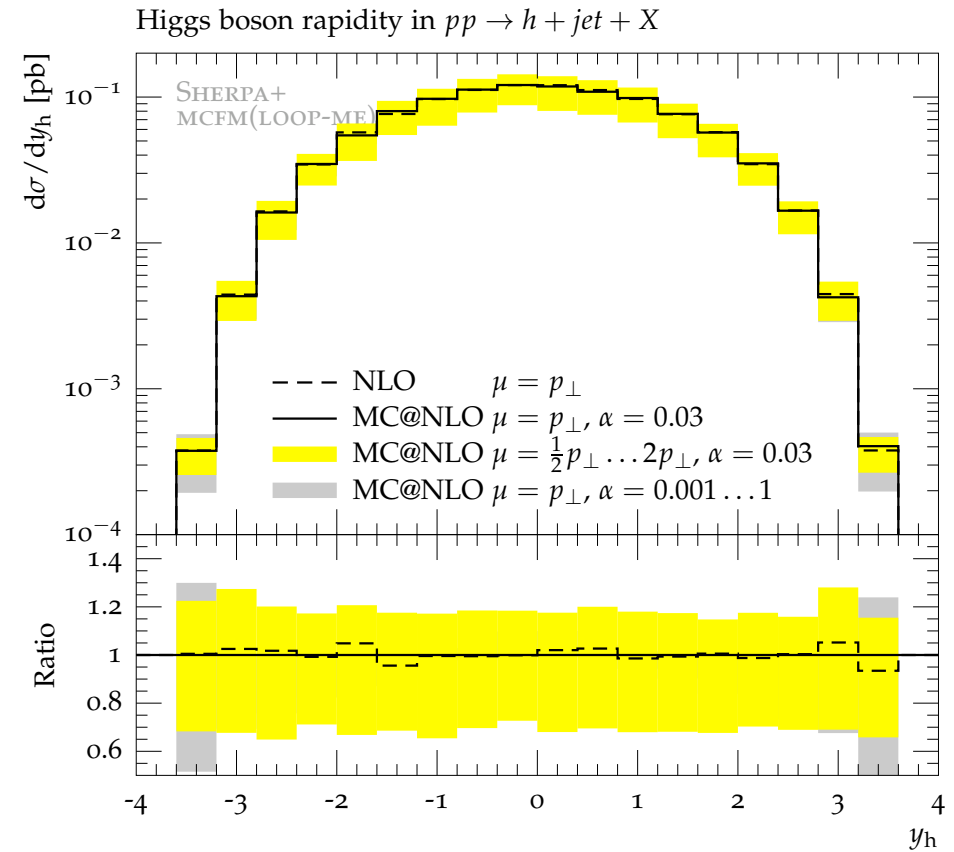
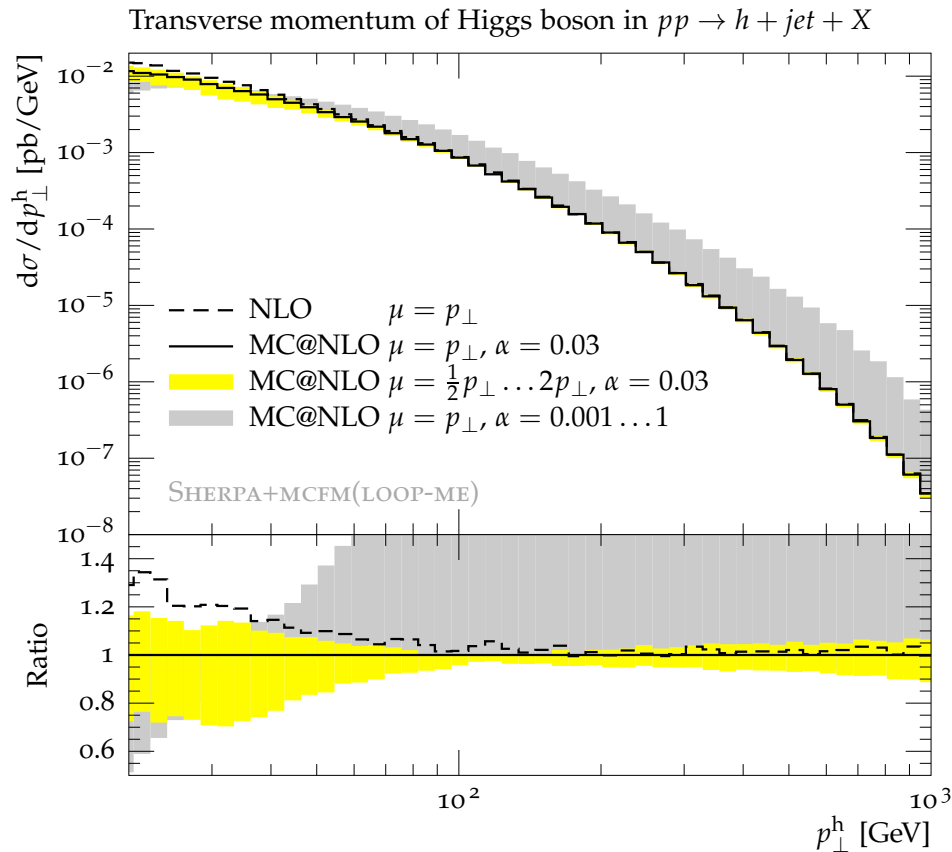
- First, NLO+PS matching needs to be under full control.
- The NLO challenge: B, V, I and S terms kinematically different from R.

# NLO+PS matching

- match **PS** to **NLO** preserving good features of both approaches  
(Sudakov suppression at small  $p_T$ , multiple soft/coll emissions)  
(NLO rate, high- $p_T$  shape, reduced scale dependence)
- matching is smooth, no phase-space separation cut, final states are ready to be hadronized
- **MC@NLO**: <http://www.hep.phy.cam.ac.uk/theory/webber/MCatNLO/>  
[FRIXIONE, WEBBER; ...]
- **aMC@NLO**: automation of MC@NLO  $\equiv$  MadFKS + MadLoop [JHEP1105(2011)044] + automation of MC subtraction terms  
[FREDERIX, FRIXIONE, TORIELLI (+ HIRSCHI, GARZELLI, MALTONI, PITTAU)] ( $W/Zb\bar{b}$  [ARXIV:1106.6019],  $Wjj$  [ARXIV:1110.5502])
- **POWHEG**: <http://powhegbox.mib.infn.it>  
[ALIOLI, HAMILTON, NASON, OLEARI, RE] ( $Vj$ /dijets [JHEP1101/4(2011)095/81],  $Wb\bar{b}$  [ARXIV:1105.4488])  
(POWHEG in Herwig/++ [RICHARDSON ET AL.] automated in Matchbox [PLÄTZER ET AL.]
- **MENLOPS**: combine POWHEG and ME+PS via phase-space slicing  
[HAMILTON, NASON, JHEP 06 (2010) 039]  
(ME+PS rescaled to correct inclusive norm by global cut-dependent  $K$ -factor.)  
(Non-unitarity of ME+PS is no problem as long as is smaller than NLO effects.)

# POWHEG and MC@NLO in Sherpa

[SLIDE FROM STEFAN HÖCHE]



Example process: Higgs-boson plus jet production at the LHC  
 Assessment of matching uncertainties in POWHEG by varying  $D^{(A)}$

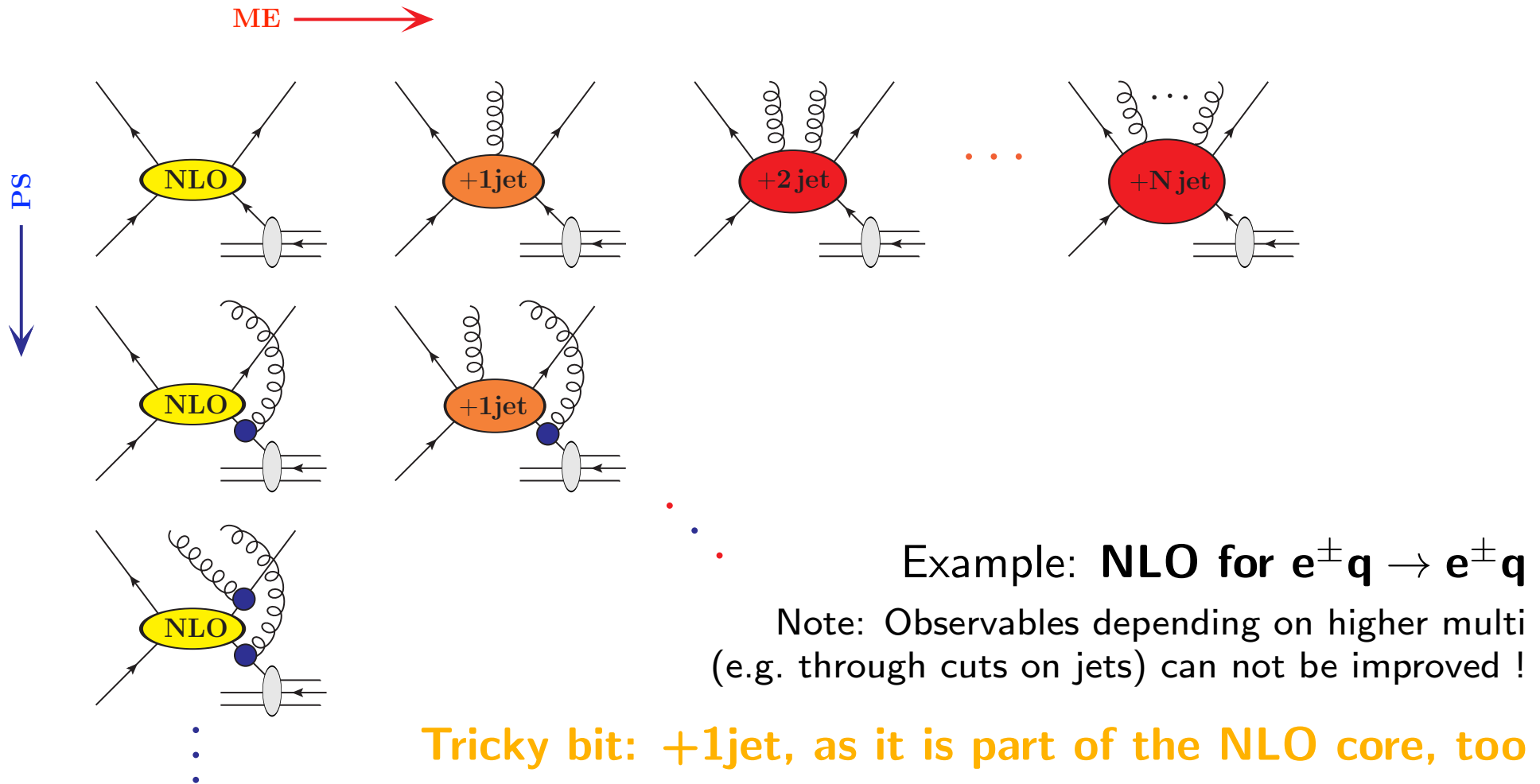
**Upper edge of band**  $\Leftrightarrow$  plain POWHEG, **lower edge**  $\Leftrightarrow$  MC@NLO

[Krauss,Schönherr,Siegert,SH] arXiv:1111.1220 [hep-ph]

**To take home:** Resumming small terms can make a big difference  
 Factorization scales must be respected in the parton shower

# MENLOPS

Promoting the simulation to NLO accuracy for the core is currently cutting edge

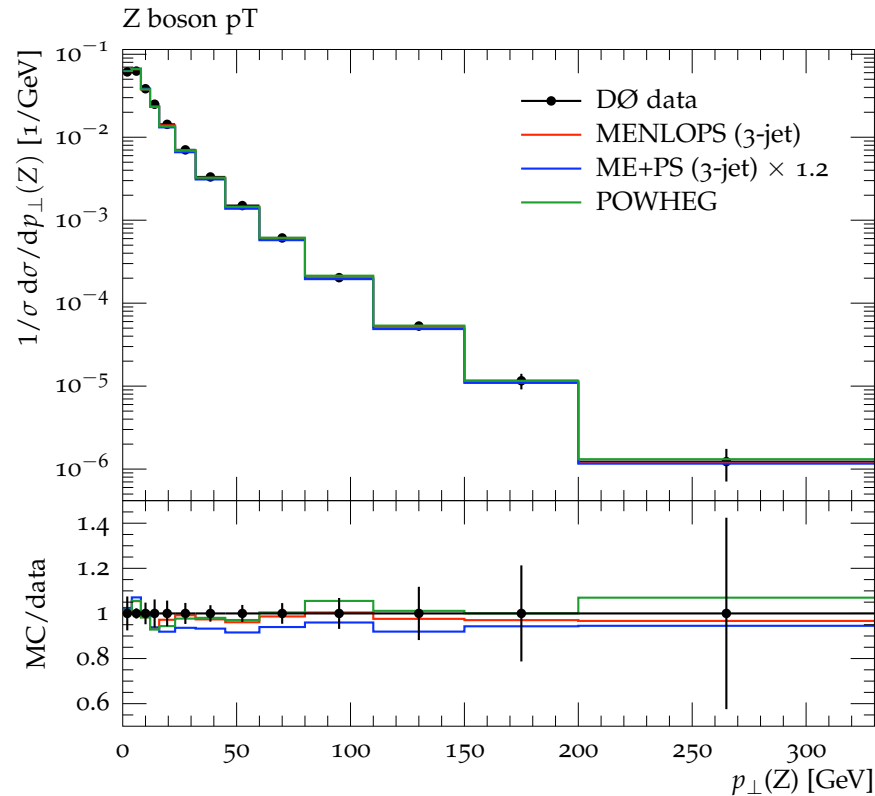


- Slice POWHEG/MC@NLO phase space in ME+PS style.

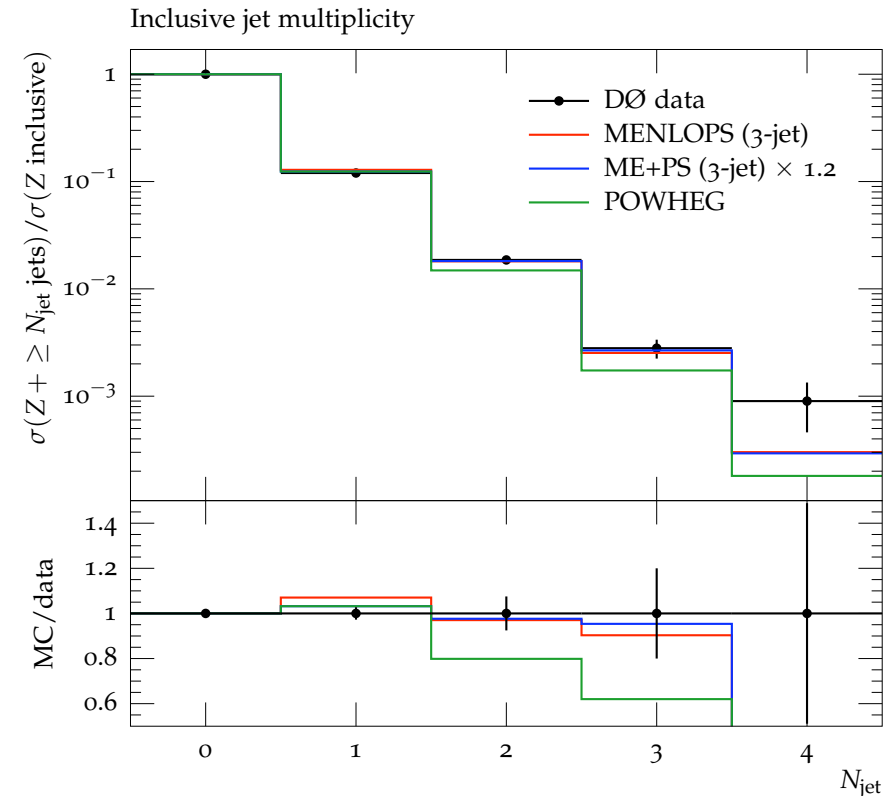
# MENLOPS in Sherpa

[HÖCHE, KRAUSS, SCHÖNHERR, SIEGERT, JHEP 08 (2011) 123]

## Z-boson $p_T$ [DØ] PLB693(2010)522



## Jet multiplicity [DØ] PLB658(2008)112



First Run II measurement using  $\mu$ 's  
Data corrected to the particle level

SHERPA prediction:  $p\bar{p} \rightarrow ll@NLO$   
 $\oplus p\bar{p} \rightarrow ll + \{1,2,3\}\text{-jets}@LO$

- accuracy inherited from POWHEG/MC@NLO  $\Rightarrow$  stable rates for core process
- higher order tree-level MEs via ME+PS  $\Rightarrow$  improved multi-jet predictions

# Summary

- Higher-order calculations are needed to meet the requirements on the precision of theoretical predictions in the LHC era.
  - Discussed by means of  $H_T$  measurements and predictions.
- Big issue is to have a very good understanding of the uncertainties related to our predictions. Necessary to have reliable estimates for  $S/B$  ratios and significances.
- Covered topics:
  - Tree-level ME+PS merging.
  - NLO exclusive sums and related problems.
  - NLO+PS matching. (new frontier  $W_{jjj}$  MC@NLO in Sherpa [ARXIV:1201.5882])
  - MENLOPS.
- Lots of subjects uncovered: needed to be selective due to short amount of time; for an extensive review of MC tools, see Phys.Rept.504(2011)145.
- Need for good understanding of how NLO, NLO+PS, ME+PS, MENLOPS and (simple) shower models compare to each other and data.
  - This is crucial for assessing any future reported anomaly.