Single top-quark production with the matrix-element method in NLO accuracy

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in collaboration with Peter Uwer

based on [JHEP 1509 (2015) 083] and ongoing work

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GRADUIERTEN KOLLEG
Masse-Spektrum-Symmetrie

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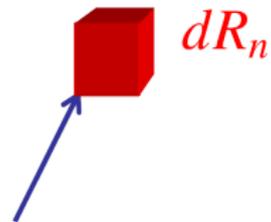# Matrix Element Method (MEM) in a nutshell [Kondo '88,'91]

For the collision $\boxed{A + B \rightarrow a_1(p_1) + a_2(p_2) + \cdots + a_n(p_n)}$

the differential cross section

$$\frac{d\sigma_n}{d^4p_1 \ldots d^4p_n} \propto \frac{1}{2s} \left| \mathcal{M}(p_1, \ldots, p_n) \right|^2 dR_n$$

$$dR_n(p_1, \ldots, p_n) = (2\pi)^4 \delta(P - \sum_i p_i) \prod_j \frac{d^3p_j}{(2\pi)^3 2E_j}$$

is a measure for the probability to observe the final state in the inf. phase space region dR_n located at $(p_1, \ldots, p_n)$

dR_n

$\vec{p} = (p_1, \ldots, p_n)$

Matrix Element Method (MEM) in a nutshell [Kondo '88,'91]

Collecting generic partonic final state variables in $\vec{x}$:

e.g. $\quad \vec{x} = (E_i, \theta_j, \dots)$: $\qquad \boxed{\dfrac{d\sigma_n}{d^4 p_1 \dots d^4 p_n} \;\rightarrow\; \dfrac{d\sigma_n}{d\vec{x}}}$

Experimentally we observe hadronic variables $\vec{y}$ instead of partonic variables $\vec{x}$.

Probability to measure $\vec{y}$:

$$\mathcal{P}(\vec{y}) = \frac{1}{\sigma} \int d\vec{x} \, \frac{d\sigma}{d\vec{x}} \, W(\vec{x}, \vec{y})$$

Transfer function $W(\vec{x}, \vec{y})$:

- ▶ Probability to experimentally observe a hadronic event $\vec{y}$ given a partonic event $\vec{x}$
- ▶ Determined by experiments through simulations
- ▶ δ-functions in the following

# Matrix Element Method (MEM) in a nutshell [Kondo '88,'91]

Extraction of model parameters Ω from data by maximizing a likelihood $\propto$ differential cross section ($\propto |\mathcal{M}^{\text{LO}}|^2$):

Likelihood as a function of Ω for event sample $\{\vec{x_i}\}$

$$\mathcal{L}^{\text{LO}}(\Omega) = \prod_i \frac{1}{\sigma^{\text{LO}}(\Omega)} \int d\vec{y} \frac{d\sigma^{\text{LO}}(\Omega)}{d\vec{y}} \underbrace{W(\vec{x_i}, \vec{y})}_{\substack{\text{transfer function,} \\ \text{here: } = \delta(\vec{x_i} - \vec{y})}} = \prod_i \frac{1}{\sigma^{\text{LO}}(\Omega)} \frac{d\sigma^{\text{LO}}(\Omega)}{d\vec{x_i}}$$

Maximizing wrt Ω yields estimator $\widehat{\Omega}$: $\quad \boxed{\mathcal{L}^{\text{LO}}(\widehat{\Omega}) = \sup_{\Omega} \mathcal{L}^{\text{LO}}(\Omega)}$

All information from event used $\implies$ most efficient estimator!
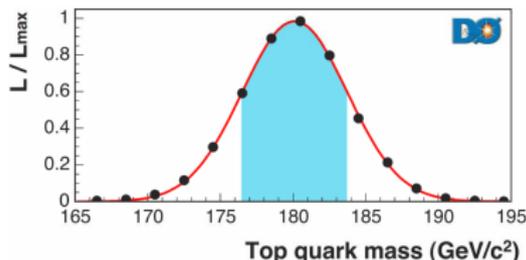
e.g. top mass measurement at Tevatron
[D0: Nature 429, 638], [CDF: PRD 50, 2966]
based on $O(70)$ events!

MEM beyond LO:

Experimental analysis so far restricted to LO

Steps towards MEM@NLO:

- ▶ Effects of real radiation [Alwall,Freitas,Mattelaer '11]

- ▶ Final states without strongly interacting particles
  [Campbell,Giele,Williams '12], [Campbell,Ellis,Giele,Williams '13]

- ▶ Steps towards final states with strongly interacting particles
  [Campbell,Giele,Williams '13]

- ▶ Complete algorithm [Martini,Uwer '15]

- ▶ Proposed generalisation [Baumeister,Weinzierl '17]

MEM beyond LO: NLO cross section at parton level

$$\sigma^{\mathsf{NLO}} = \overbrace{\int dR_n \frac{d\sigma^{\mathsf{B}}}{dR_n}}^{\text{Born}} + \underbrace{\overbrace{\int dR_n \frac{d\sigma^{\mathsf{V}}}{dR_n}}^{\text{virtual}} + \overbrace{\int dR_{n+1} \frac{d\sigma^{\mathsf{R}}}{dR_{n+1}}}^{\text{real}}}_{\text{separately IR divergent}}$$
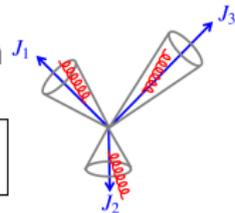
Jet Physics: observed final states are jets

partonic events $\longrightarrow$ "Jet events"

New in NLO:

- Infrared and collinear divergences in virtual and real corrections $\xrightarrow{\text{KLN theorem}}$ mutual cancelation

- $n+1$ particle phase space due to real corrections: Non-trivial mapping: parton momenta $\leftrightarrow$ jet momenta

Born and virtual: $J_i = p_i$ trivial but real: $J_i = \widetilde{J}_i(p_1, \dots, p_{n+1})$

Likelihood at NLO: 3 major obstacles

$$\mathcal{L}^{\text{NLO}}(\Omega) = \prod_i \frac{1}{\sigma_{n\text{-jet}}^{\text{NLO}}(\Omega)} \left(\frac{d\sigma_{n\to n\text{-jet}}^{\text{B+V}}(\Omega)}{dJ_1 \ldots dJ_n} + \frac{d\sigma_{n+1\to n\text{-jet}}^{\text{R}}(\Omega)}{dJ_1 \ldots dJ_n} \right)\Bigg|_{\text{event } i}$$
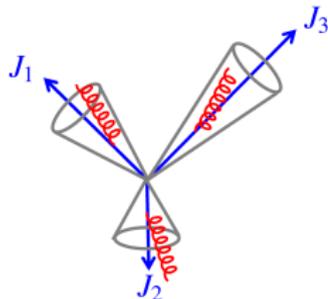
- ▶ Born+virtual and real contribution separately IR divergent

  NEED: Point-wise cancelation in jet phase space

- ▶ Integration over jet cones in real contribution introduces δ-functions → numerically problematic!

  NEED: factorisation of real phase space

- ▶ Born+virtual matrix elements only defined for 'Born kinematics'

  NEED: clustered jets obeying 'Born kinematics'

Proposal: Replace $2 \to 1$ clustering by $3 \to 2$ clustering

$3 \to 2$ clustering $p_i, p_j, p_k \to \widetilde{J}_{ij}, \widetilde{J}_k$
can meet all 3 requirements at the same time

$\Downarrow$

Using $3 \to 2$ jet algorithm instead of $2 \to 1$
allows to overcome the 3 obstacles

$3 \to 2$ clusterings inspired by Catani-Seymour dipole subtraction method [Catani, Seymour '97], [Catani, Dittmaier, Seymour, Trocsanyi '02]

Jet event weight at NLO

Phase space factorisation allows to define an event weight
(differential jet cross section) at NLO

$$\frac{d\sigma_{n\text{-jet}}^{\text{NLO}}(\Omega)}{dJ_1 \ldots dJ_n} = \underbrace{\frac{d\sigma^{\text{B+V}}(\Omega)}{dJ_1 \ldots dJ_n}}_{\text{still IR divergent}} + \underbrace{\overbrace{\int dR_{\text{unres}}(\Phi)}^{\text{3dim integration}} \frac{d\sigma^{\text{R}}(\Omega)}{dp_1 \ldots dp_{n+1}}}_{\text{still IR divergent}}$$

$$\underbrace{}_{\text{finite through subtraction/slicing}}$$

Mutual cancelation of IR-divergences from the virtual and the real
part has to be carried out by a suitable method (e.g. phase space
slicing)

Validation

We consider the s–channel or t–channel production of single top quarks in association with a light jet at the LHC

$$p + p \to t + j \, (+X) \quad @ \text{ NLO QCD}$$

optional veto on additional jet emission!

Note: top decay not included, tops are treated as tagged top jets

To Check:

1. Generation of real phase space
2. Generation of unweighted events (at NLO accuracy!)

Validation 1: Phase space generation

Calculate jet distributions in NLO accuracy using conventional approach (parton level MC + $3 \to 2$ jet alg.) and compare with distributions obtained from $\frac{d\sigma_{n\text{-jet}}^{\text{NLO}}(\Omega)}{dJ_1 \ldots dJ_n}$ with factorised jet phase space

s-channel single top $pp \to tj$, $\sqrt{s} = 13$ TeV,
exclusive $kt_{3\to2}$-Alg. (min. spectator infl.),
$p^{\perp} > \sqrt{d_{\text{cut}}} = 30$ GeV, $|\eta| < 3.5$

conventional PS
factorised jet PS

p-val=0.40, χ^2_{red}=1.05
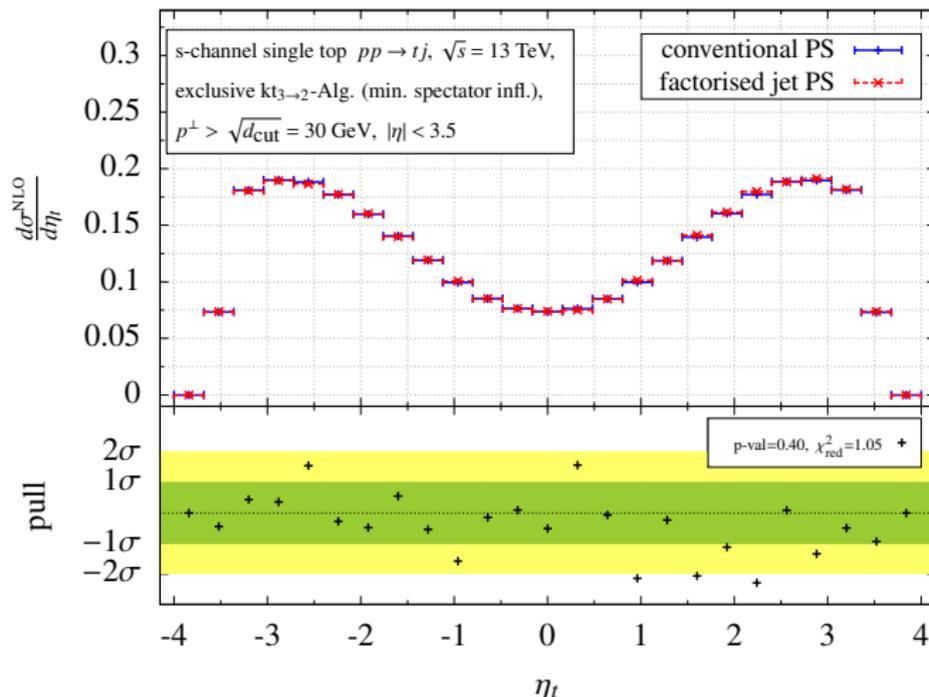
Validation 2: Unweighted events

Fill histograms with unweighted events generated according to $\rho = \frac{d\sigma_{n\text{-jet}}^{\text{NLO}}(\Omega)}{dJ_1...dJ_n}$ and compare with jet distributions in NLO accuracy obtained from conventional approach (parton MC + $3 \to 2$ clus.)
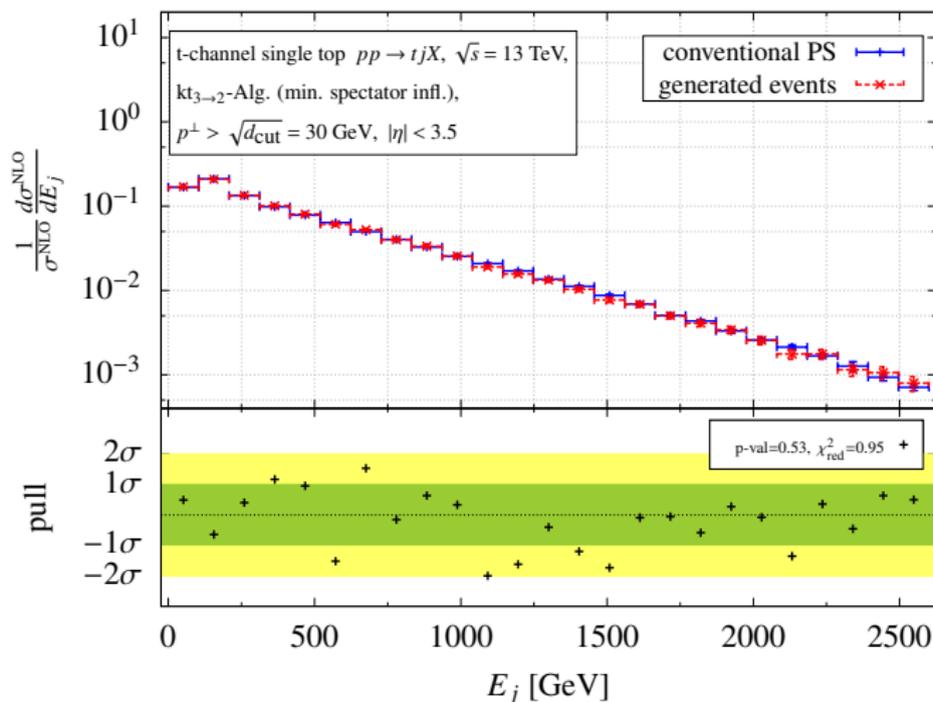
Application: Matrix Element Method at NLO

(example: $p + p \rightarrow t + j$ via s-/t-channel @ NLO QCD)

Toy experiment: Generate sample of N unweighted NLO tj events

$$\vec{x}_i = (\eta_t, E_j, \eta_j, \phi_j)_i \quad \text{with } \Omega = m_t = m_t^{\text{true}} = 173.2 \text{ GeV}$$

NLO likelihood function for event sample

$$\mathcal{L}^{\text{NLO}}(m_t) = \prod_i^N \mathcal{L}^{\text{NLO}}(\vec{x}_i | m_t) = \left(\frac{1}{\sigma^{\text{NLO}}(m_t)} \right)^N \prod_{i=1}^N \left(\frac{E_j^2 \cosh(\eta_t)}{2 \, s \, E_t \, \cosh^3(\eta_j)} \, \frac{d\sigma^{\text{NLO}}}{d^4 J_t \, d^4 J_j}(m_t) \right) \Bigg|_i$$

Find minimum of negative logarithm of NLO likelihood
("Log-Likelihood") to obtain estimator $\widehat{m}_t$ for top mass

$$-\log \mathcal{L}^{\text{NLO}}(\widehat{m}_t) = \inf_{m_t} \left(-\log \mathcal{L}^{\text{NLO}}(m_t) \right)$$

MEM at NLO: s-channel, no veto on additional jet

s-channel single top $pp \to tjX$, $\sqrt{s} = 13$ TeV,

$kt_{3\to2}$-Alg. (min. spectator infl.),

$p^\perp > \sqrt{d_{\text{cut}}} = 30$ GeV, $|\eta| < 3.5$,

16964 NLO s-channel single top events,

Fit: $f(m_t) = -\log \mathcal{L}_{\min} + \left(\frac{m_t - \widetilde{m}_t}{\sqrt{2}\,\Delta\widetilde{m}_t}\right)^2$,

$\widetilde{m}_t^{\text{NLO}} \pm \Delta\widetilde{m}_t^{\text{NLO}} = (173.07^{-1.61}_{+2.32} \pm 0.90^{+0.01}_{+0.09})$ GeV,

$\widetilde{m}_t^{\text{Born}} \pm \Delta\widetilde{m}_t^{\text{Born}} = (171.01^{+2.42}_{-2.89} \pm 0.92^{+0.02}_{-0.01})$ GeV

Legend:
- Born, $\mu_0/2$
- Born, μ_0
- Born, $2\mu_0$
- NLO, $\mu_0/2$
- NLO, μ_0
- NLO, $2\mu_0$
- $m_t^{\text{true}} = 173.2$ GeV
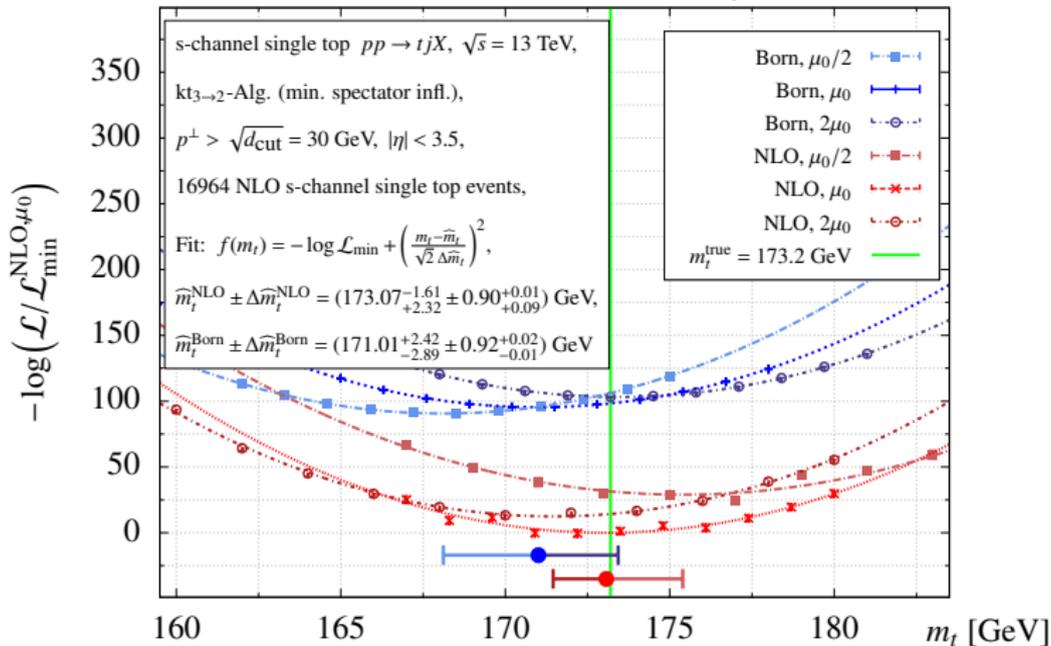
NLO analysis recovers m_t^{true} but biased if MEM@LO is used!

▶ $\approx 17k$ events allow already precise mass determination

▶ Impact of scale variation reduced in NLO analysis

▶ Bias in LO estimator covered by scale variation between $[\frac{\mu_0}{2}, 2\mu_0]$

MEM at NLO: t-channel, veto on additional jet

t-channel single top $pp \to tj$, $\sqrt{s} = 13$ TeV,

exclusive $kt_{3\to2}$-Alg. (min. spectator infl.),

$p^\perp > \sqrt{d_{\text{cut}}} = 30$ GeV, $|\eta| < 3.5$,

24088 NLO t-channel single top events,

Fit: $f(m_t) = -\log \mathcal{L}_{\min} + \left(\frac{m_t - \widetilde{m}_t}{\sqrt{2}\,\Delta\widetilde{m}_t} \right)^2$,

$\widetilde{m}_t^{\text{NLO}} \pm \Delta\widetilde{m}_t^{\text{NLO}} = (173.79^{-1.84}_{+2.78} \pm 1.62^{-0.05}_{-0.06})$ GeV,

$\widetilde{m}_t^{\text{Born}} \pm \Delta\widetilde{m}_t^{\text{Born}} = (160.74^{+6.21}_{-7.70} \pm 1.68^{+0.01}_{-0.01})$ GeV,

Legend:
- Born, $\mu_0/2$
- Born, μ_0
- Born, $2\mu_0$
- NLO, $\mu_0/2$
- NLO, μ_0
- NLO, $2\mu_0$
- $m_t^{\text{true}} = 173.2$ GeV
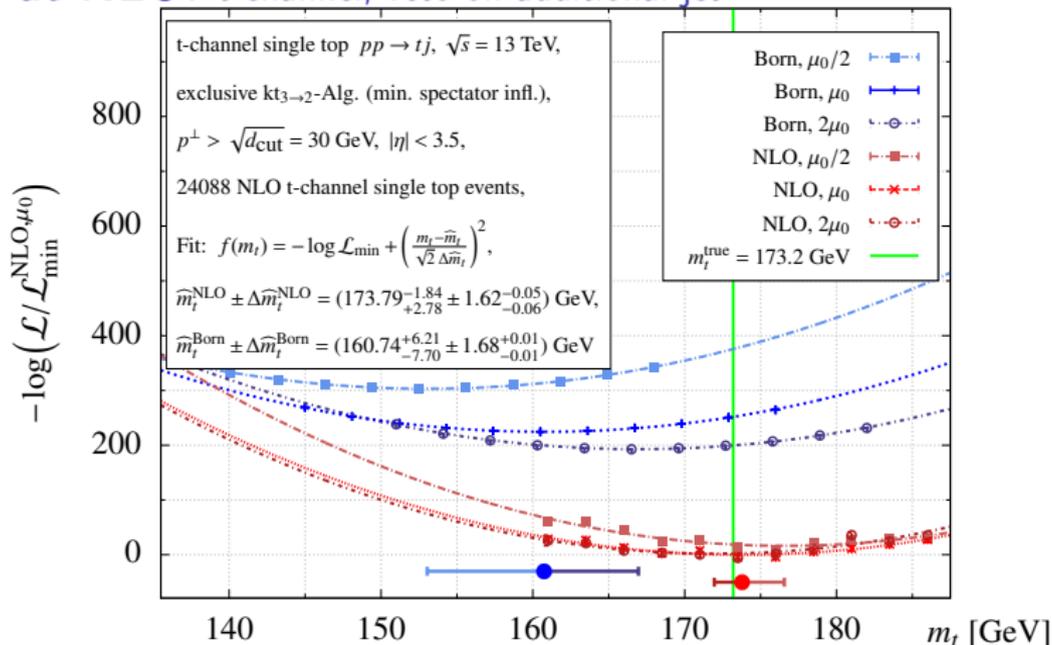
NLO analysis recovers m_t^{true} but biased if MEM@LO is used!

- ▶ Impact of scale variation significantly reduced in NLO analysis
- ▶ Shift in LO analysis not covered by scale variation ⇒ naive variation between $[\frac{\mu_0}{2}, 2\mu_0]$ in LO analysis may not give reliable estimate of NLO effects
- ▶ Large shift observed in LO analysis would require significant calibration with related uncertainties

Conclusion

$3 \rightarrow 2$ jet clustering algorithm:

- ▶ Uniquely maps real corrections onto Born kinematics

Allows:

- ▶ Evaluation of event weights for jet events in NLO accuracy

- ▶ Generation of unweighted events at NLO

- ▶ Application of MEM at NLO
    - ▶ Extraction of m_t with NLO likelihood from NLO single top events: Perfect agreement with input value!
    - ▶ Extraction with Born likelihood: Large deviation from input value possible (not necessarily covered by scale variation)!
    - ▶ Renormalization scheme well-defined in MEM at NLO (extracted mass = pole mass)

Outlook: MEM at NLO for top+Higgs

BackUp: Ingredients of iterative $2 \to 1$ jet algorithms

1. Resolution:
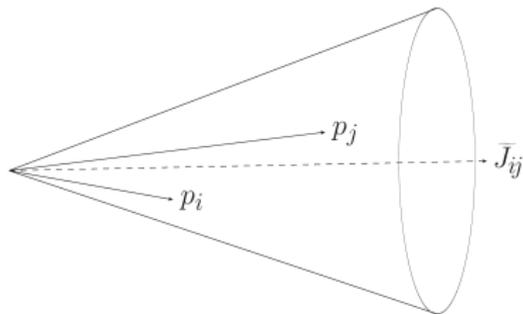
e.g.
$$y_{ij} = \min(p_i^{\perp 2p}, p_j^{\perp 2p}) \frac{\Delta_{ij}}{R^2}, \quad \Delta_{ij} = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$

($p = 1$: "kt-algorithm", $p = -1$: "anti-kt-algorithm")

2. Recombination/Clustering:

If $y_{ij} < y_{\text{cut}}$:
p_i, p_j are clustered to jet $\widetilde{J}_{ij}$

e.g.
$$\boxed{\widetilde{J}_{ij} = p_i + p_j}$$

$\to$ respects 4-momentum conservation, violates on-shell condition

or
$$\boxed{\widetilde{\vec{J}}_{ij} = \vec{p}_i + \vec{p}_j, \quad \widetilde{J}_{ij}^0 = \sqrt{\widetilde{\vec{J}}_{ij}^2 + m_{ij}^2}}$$

$\to$ respects on-shell condition, violates energy conservation

("p-scheme")

BackUp: $3 \to 2$ jet algorithm as an augmented $2 \to 1$ algorithm

- Use resolution criterium y_{ij} of the $2 \to 1$ algorithm to pick final state particle to be clustered with final state particle or beam ("emitter")

- Choose final state particle or beam as "spectator"

- 4 different types of mappings
  (emitter,spectator) = (final,final), (final,initial), (initial, initial), (initial,final)

- Respective clusterings for massless and massive particles already worked out in Catani-Seymour dipole subtraction method [Catani,Seymour '97], [Catani,Dittmaier,Seymour,Trocsanyi '02] (let's use those!)
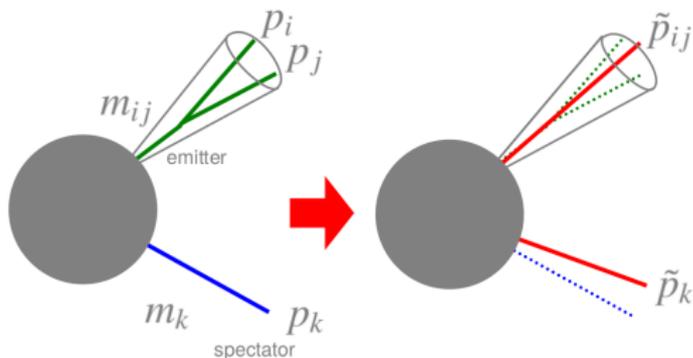
BackUp: Modified clustering

[Catani,Seymour '97], [Catani,Dittmaier,Seymour,Trocsanyi '02]

(example: massless final state clustering with final state spectator)

$$(p_i, p_j, p_k) \to \left(\widetilde{p}_{ij} = p_i + p_j - \frac{y}{1-y} p_k, \ \widetilde{p}_k = \frac{1}{1-y} p_k \right) \to (\widetilde{J}_{ij}, \widetilde{J}_k)$$

$$\widetilde{J}_{ij} + \widetilde{J}_k = p_i + p_j + p_k$$

and $\widetilde{J}_{ij}^2 = m_{ij}^2, \ \widetilde{J}_k^2 = m_k^2$

Phase space factorises: $dR_{n+1}(p_i, p_j, p_k) = dR_n(\widetilde{J}_{ij}, \widetilde{J}_k) dR_{\text{unres}}(\Phi)$

integrating over $dR_{\text{unres}}(\Phi = \{\phi, z, y\}) = \frac{\widetilde{J}_{ij} \cdot \widetilde{J}_k}{2(2\pi)^3} \ d\phi \ dz \ dy \ (1-y)$

generates all p_i, p_j, p_k with $(p_i, p_j, p_k) \overset{!}{\to} (\widetilde{J}_{ij}, \widetilde{J}_k)$

BackUp: Modified clustering: Generation of real phase space

(e.g. massless final-final clustering à la Catani-Seymour)

3→2 jet clustering: $\boxed{(p_1, ..., p_{n+1}) \to (\widetilde{J}_1, ..., \widetilde{J}_n, \Phi)}$

$\widetilde{J}_{ij} = p_i + p_j - \frac{y}{1-y} p_k, \qquad \widetilde{J}_k = \frac{1}{1-y} p_k, \qquad \widetilde{J}_m = p_m, \ m \neq i, j, k$

$\Phi = \left\{ \phi, \ z = \frac{p_i \cdot p_k}{p_k \cdot (p_i + p_j)}, \ y = \frac{p_i \cdot p_j}{p_i \cdot p_j + p_k \cdot (p_i + p_j)} \right\}$

Opposite direction required: $\boxed{(\widetilde{J}_1, ..., \widetilde{J}_n, \Phi) \to (p_1, ..., p_{n+1})}$
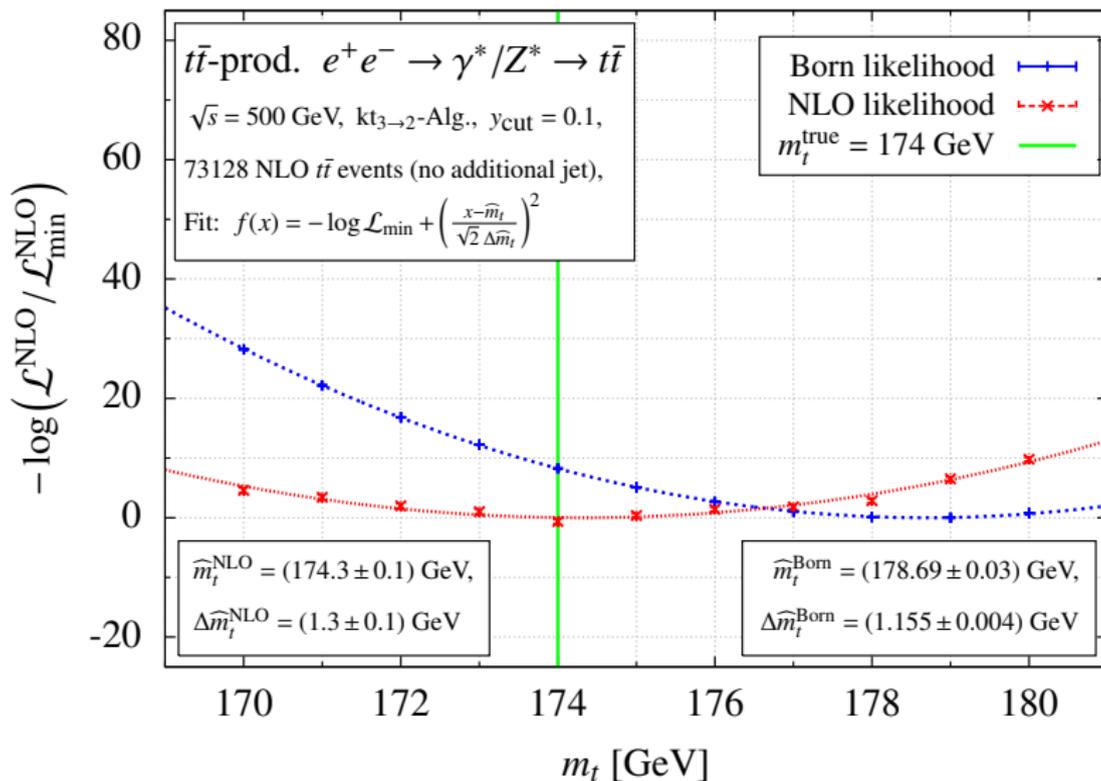
$p_i + p_j = \widetilde{J}_{ij} + y \widetilde{J}_k, \qquad p_k = (1-y) \widetilde{J}_k, \qquad p_m = \widetilde{J}_m, \ m \neq i, j, k$

$\Phi = \left\{ \phi, \ z = \frac{p_i \cdot \widetilde{J}_k}{\widetilde{J}_{ij} \cdot \widetilde{J}_k}, \ y = \frac{p_i \cdot p_j}{\widetilde{J}_{ij} \cdot \widetilde{J}_k} \right\}$

Phase space factorises: $\boxed{dR_{n+1}(p_1, ..., p_{n+1}) = dR_n(\widetilde{J}_1, \ldots, \widetilde{J}_n) dR_{\text{unres}}(\Phi)}$

$\implies \quad dR_{\text{unres}} \longrightarrow \left(p_1(\widetilde{J}_1, \ldots, \widetilde{J}_n, \Phi), \ldots, p_{n+1}(\widetilde{J}_1, \ldots, \widetilde{J}_n, \Phi) \right)$

BackUp: MEM at NLO: top-quark mass extraction from $e^+e^- \to t\bar{t}$

$t\bar{t}$-prod. $e^+e^- \to \gamma^*/Z^* \to t\bar{t}$

$\sqrt{s} = 500$ GeV, $kt_{3\to2}$-Alg., $y_{cut} = 0.1$,

73128 NLO $t\bar{t}$ events (no additional jet),

Fit: $f(x) = -\log \mathcal{L}_{min} + \left(\frac{x - \widehat{m}_t}{\sqrt{2}\,\Delta\widehat{m}_t}\right)^2$

Born likelihood

NLO likelihood

$m_t^{true} = 174$ GeV

$\widehat{m}_t^{NLO} = (174.3 \pm 0.1)$ GeV,

$\Delta\widehat{m}_t^{NLO} = (1.3 \pm 0.1)$ GeV

$\widehat{m}_t^{Born} = (178.69 \pm 0.03)$ GeV,

$\Delta\widehat{m}_t^{Born} = (1.155 \pm 0.004)$ GeV

Axis labels: $-\log\left(\mathcal{L}^{NLO}/\mathcal{L}_{min}^{NLO}\right)$ versus m_t [GeV]

NLO analysis recovers m_t^{true} but significant difference if MEM@LO is used!