On the ambiguities of the BLM/PMC procedure for hadron collider processes

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based on 1907.06610 with A. Mitov
1. Introduction

2. BLM/PMC procedure and $t\bar{t}$ production
   - Introduction to the BLM/PMC procedure
   - Ambiguities in the BLM/PMC procedure
   - $t\bar{t}$ production at NNLO

3. Results
   - PMC scales
   - Hadronic cross-sections at Tevatron and at LHC
   - Impact of ambiguities
   - Comparison of strategies to handle the $q_4$ ambiguity

4. Conclusion
Renormalisation scale, $\mu_R$

- Observables in perturbative QCD:
  \[ \sum_n C_n(\mu_R) \alpha_s^n(\mu_R) \]
- In finite order calculations, observables become dependent on $\mu_R$
- Value of $\mu_R$ is arbitrary
Estimating theoretical uncertainties

• Observables in perturbative QCD:

\[ \sum_n C_n(\mu_R) \alpha_s^n(\mu_R) \]

• In practical calculations, theoretical uncertainties arise from neglecting higher-order terms.

• Conventionally, vary value of \( \mu_R \) to estimate size of the theoretical uncertainties

• Scale-setting methods cannot fully remove the uncertainty arising from neglected higher-order terms.
\[ a_s(\mu_R) = \frac{\alpha_s(\mu_R)}{4\pi} \]

\[ \mu_R^2 \frac{\partial a_s(\mu_R)}{\partial \mu_R^2} = -\beta_0 a_s^2 - \beta_1 a_s^3 - \beta_2 a_s^4 - \ldots \]

\[ \beta_0 = 11 - \frac{2}{3} n_f \]

\[ \beta_1 = 102 - \frac{38}{3} n_f \]

\[ a_s(\mu_2) = a_s(\mu_1) - \beta_0 L a_s^2(\mu_1) + \left( \beta_0^2 L^2 - \beta_1 L \right) a_s^3(\mu_1) + O(a_s^4) \]

where \( L := \log(\mu_2^2/\mu_1^2) \)
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Conformal symmetry

- Without quark masses, QCD Lagrangian is conformally-invariant.
- Running of $\alpha_s$ introduces a mass scale $\Lambda_{QCD}$ and breaks conformal symmetry.
- In the perturbative expansion of an observable, $\sum_n C_n \alpha_s^n$, the coefficients $C_n$ contain the $\beta$-function coefficients $\beta_i$.
- Principle of Maximum Conformality: choose $\mu_R$ such that the $\beta_i$ terms in $C_n$ get absorbed into the running coupling.
- NB: In practice, identify $\beta_i$-dependence of $C_n$ via $n_f$ dependence.
BLM/PMC scale setting: NLO
(Brodsky, Lepage, Mackenzie; 1983)

\[ \sigma = c_2 a_s^2(\mu_R) + c_3 (\mu_R) a_s^3(\mu_R) \]
\[ \equiv s_{2,0} a_s^2(\mu_R) + \left[ s_{3,0} + 2 \beta_0 s_{3,1}(\mu_R) \right] a_s^3(\mu_R) \]

Recall: \[ a_s(\mu_2) = a_s(\mu_1) - \beta_0 \log \left( \frac{\mu_2^2}{\mu_1^2} \right) a_s^2(\mu_1) + \mathcal{O}(a_s^3) \]

Can absorb \( \beta_0 \) term by choosing scale \( \mu_{BLM} \):

\[ \log \left( \frac{\mu_{BLM}^2}{\mu_R^2} \right) = - \frac{s_{3,1}(\mu_R)}{s_{2,0}} \]

\[ \sigma_{BLM} = s_{2,0} a_s^2(\mu_{BLM}) + s_{3,0} a_s^3(\mu_{BLM}) \]
At NNLO, one cannot in general absorb all $\beta_i$ terms with a single choice of scale.

$$
\sigma = s_{2,0} a_s^2 (\mu_R) \\
+ \left[ s_{3,0} + 2 s_{3,1} (\mu_R) \beta_0 \right] a_s^3 (\mu_R) \\
+ \left[ s_{4,0} + 2 s_{3,1} (\mu_R) \beta_1 + 3 s_{4,1} (\mu_R) \beta_0 + 3 s_{4,2} (\mu_R) \beta_0^2 \right] a_s^4 (\mu_R)
$$

The PMC proposes using a different scale at each order of $\alpha_s$, while maintaining consistency with the renormalisation group

$$
\sigma_{PMC} = s_{2,0} a_s^2 (q_2) + s_{3,0} a_s^3 (q_3) + s_{4,0} a_s^4 (q_4)
$$

$$
\log \left( \frac{q_2^2}{\mu_R^2} \right) = - \frac{s_{3,1}}{s_{2,0}} + \frac{3}{2} \left[ \left( \frac{s_{3,1}}{s_{2,0}} \right)^2 - \frac{s_{4,2}}{s_{2,0}} \right] \beta_0 a_s(\mu_R)
$$

$$
\log \left( \frac{q_3^2}{\mu_R^2} \right) = - \frac{s_{4,1}}{s_{3,0}}
$$

$q_4 = q_3$
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4. Conclusion
Ambiguities in BLM/PMC procedure

- At NNLO, one cannot in general absorb all $\beta_i$ terms with a single choice of scale.

$$\sigma = s_{2,0} a_s^2(\mu_R)$$
$$\quad + \left[ s_{3,0} + 2 s_{3,1} (\mu_R) \beta_0 \right] a_s^3(\mu_R)$$
$$\quad + \left[ s_{4,0} + 2 s_{3,1} (\mu_R) \beta_1 + 3 s_{4,1} (\mu_R) \beta_0 + 3 s_{4,2} (\mu_R) \beta_0^2 \right] a_s^4(\mu_R)$$

- The PMC proposes using a different scale at each order of $\alpha_s$, while maintaining consistency with the renormalisation group.

$$\sigma_{PMC} = s_{2,0} a_s^2(q_2) + s_{3,0} a_s^3(q_3) + s_{4,0} a_s^4(q_4)$$

$$\log \left( \frac{q_2^2}{\mu^2_R} \right) = -\frac{s_{3,1}}{s_{2,0}} + \frac{3}{2} \left[ \left( \frac{s_{3,1}}{s_{2,0}} \right)^2 - \frac{s_{4,2}}{s_{2,0}} \right] \beta_0 a_s(\mu_R)$$

$$\log \left( \frac{q_3^2}{\mu^2_R} \right) = -\frac{s_{4,1}}{s_{3,0}}$$

($q_4 = q_3$)
At NNLO, one cannot in general absorb all $\beta_i$ terms with a single choice of scale.

$$\sigma = s_{2,0} a_s^2(\mu_R) + \left[ s_{3,0} + 2s_{3,1}(\mu_R) \beta_0 \right] a_s^3(\mu_R) + \left[ s_{4,0} + 2s_{3,1}(\mu_R) \beta_1 + 3s_{4,1}(\mu_R) \beta_0 + 3s_{4,2}(\mu_R) \beta_0^2 \right] a_s^4(\mu_R)$$

The PMC proposes using a different scale at each order of $\alpha_s$, while maintaining consistency with the renormalisation group

$$\sigma_{PMC} = s_{2,0} a_s^2(q_2) + s_{3,0} a_s^3(q_3) + s_{4,0} a_s^4(q_4)$$

$$\log \left( \frac{q_2'}{\mu_R^2} \right) = -\frac{s_{3,1}}{s_{2,0}}$$

$$\log \left( \frac{q_3'}{\mu_R^2} \right) = -\frac{s_{4,1}}{s_{3,0}} + \frac{s_{2,0}}{s_{3,0}} \left[ \left( \frac{s_{3,1}}{s_{2,0}} \right)^2 - \frac{s_{4,2}}{s_{2,0}} \right] \beta_0$$

$$(q_4 = q_3)$$
Summary of ambiguities

\[ \sigma_{PMC} = s_{2,0} a_s^2(q_2) + s_{3,0} a_s^3(q_3) + s_{4,0} a_s^4(q_4) \]

1. **Choice of initial scale \( \mu_R \)**

\[
\log \left( \frac{q_2^2}{\mu_R^2} \right) = -\frac{s_{3,1}}{s_{2,0}} + \frac{s_3}{3} \left[ \left( \frac{s_{3,1}}{s_{2,0}} \right)^2 - \frac{s_{4,2}}{s_{2,0}} \right] \beta_0 a_s(\mu_R)
\]

\[
\log \left( \frac{q_3^2}{\mu_R^2} \right) = -\frac{s_{4,1}}{s_{3,0}}
\]

2. **Choice of highest PMC scale \( q_4 \)**

3. **Use of \( q_n \) vs \( q'_n \)**

\[
\log \left( \frac{q_2^{'2}}{\mu_R^2} \right) = -\frac{s_{3,1}}{s_{2,0}}
\]

\[
\log \left( \frac{q_3^{'2}}{\mu_R^2} \right) = -\frac{s_{4,1}}{s_{3,0}} + \frac{s_{2,0}}{s_{3,0}} \left[ \left( \frac{s_{3,1}}{s_{2,0}} \right)^2 - \frac{s_{4,2}}{s_{2,0}} \right] \beta_0
\]
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**tt̄ production at NNLO**

- **Partonic cross-section:** \( \sigma_{ij \rightarrow t\bar{t} + X} = C_2 \alpha_s^2 + C_3 \alpha_s^3 + C_4 \alpha_s^4 + \ldots \)

- **6 channels:**
  - **LO:** \( q\bar{q} \) and \( gg \)
  - **NLO:** \( gq \)
  - **NNLO:** \( qq, q\bar{q}', q\bar{q}' \)

- **Define kinematic variable** \( v = \sqrt{1 - 4m_t^2/\hat{s}} \)

- **\( \mu_F \) fixed at \( m_t \)**

- **PMC applied to \( q\bar{q} \) and \( gg \) channels (separately)**

- **PMC scales (\( q_n \)) and coefficients (\( s_{n,k} \)) are \( v \)-dependent**

- **Hadronic cross-sections computed by convolving partonic cross-sections with PDFs (here NNPDF3.1)**

- **Caveat:** In \( gg \) channel, \( C_4 \) has \( n_f \) contributions from “light-by-light” scattering diagrams. In principle, these should not be absorbed into the running coupling.
Coulomb terms

- At low $\nu$, $t\bar{t}$ try to form bound states
- Beyond $N^3LO$, partonic cross-section has non-integrable $\frac{1}{\sqrt{n}}$ singularities ("Coulomb terms")
- In principle, should resum Coulomb terms
- Relevance to PMC: we will separate Coulomb and non-Coulomb terms. We apply the PMC to only the non-Coulomb terms.
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PMC scale $q_2$ for $q\bar{q}$ channel

$$\sigma_{PMC} = s_{2,0} a_s^2(q_2) + s_{3,0} a_s^3(q_3) + s_{4,0} a_s^4(q_4)$$
Results

PMC scales

PMC scale $q_3$ for $q\bar{q}$ channel

$$\sigma_{PMC} = s_{2,0}a_s^2(q_2) + s_{3,0}a_s^3(q_3) + s_{4,0}a_s^4(q_4)$$

![Graph showing $q_3$ and $q'_3$]
PMC scale $q_2$ for $gg$ channel

$$\sigma_{PMC} = s_{2,0}a_s^2(q_2) + s_{3,0}a_s^3(q_3) + s_{4,0}a_s^4(q_4)$$
PMC scale $q_3$ for $gg$ channel

\[ \sigma_{PMC} = s_{2,0} a_s^2(q_2) + s_{3,0} a_s^3(q_3) + s_{4,0} a_s^4(q_4) \]
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4. Conclusion
Table: Contribution of the $q\bar{q}$ and $gg$ channels to $\sigma_{p\bar{p} \rightarrow t\bar{t} + X}$ at the Tevatron

<table>
<thead>
<tr>
<th></th>
<th>$q\bar{q}$ channel</th>
<th>$gg$ channel</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PMC [pb]</td>
<td>Conv. [pb]</td>
</tr>
<tr>
<td>$\alpha_s^2$</td>
<td>4.55</td>
<td>4.89</td>
</tr>
<tr>
<td>$\alpha_s^3$</td>
<td>3.31</td>
<td>0.96</td>
</tr>
<tr>
<td>$\alpha_s^4$</td>
<td>-2.24</td>
<td>0.42</td>
</tr>
<tr>
<td>NNLO [pb]</td>
<td>5.62</td>
<td>$6.27^{+0.16}_{-0.20}$</td>
</tr>
<tr>
<td></td>
<td>PMC [pb]</td>
<td>Conv. [pb]</td>
</tr>
<tr>
<td>$\sigma_{BLM/PMC}$ ($p\bar{p} \rightarrow t\bar{t}$)</td>
<td>6.48 pb</td>
<td></td>
</tr>
<tr>
<td>$\sigma_{Conventional}$ ($p\bar{p} \rightarrow t\bar{t}$)</td>
<td>7.06$^{+0.21}_{-0.25}$ pb</td>
<td></td>
</tr>
<tr>
<td>$\sigma_{Experimental}$ ($p\bar{p} \rightarrow t\bar{t}$)</td>
<td>7.60 ± 0.41 pb</td>
<td></td>
</tr>
</tbody>
</table>

$\sigma_{Exp.}$: Phys. Rev. D 89 (2014) 072001
Hadronic cross-section at LHC

**Table:** Contribution of the $q\bar{q}$ and $gg$ channels to $\sigma_{pp \rightarrow t\bar{t} + X}$ at the 13 TeV LHC

<table>
<thead>
<tr>
<th></th>
<th>$q\bar{q}$ channel</th>
<th>$gg$ channel</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PMC</td>
<td>Conv.</td>
</tr>
<tr>
<td>$\alpha_s^2$ [pb]</td>
<td>62.4</td>
<td>68.5</td>
</tr>
<tr>
<td>$\alpha_s^3$ [pb]</td>
<td>41.7</td>
<td>8.5</td>
</tr>
<tr>
<td>$\alpha_s^4$ [pb]</td>
<td>-32.3</td>
<td>4.7</td>
</tr>
<tr>
<td>NNLO [pb]</td>
<td>71.8</td>
<td>$81.8^{+1.9}_{-2.2}$</td>
</tr>
</tbody>
</table>

\[
\sigma_{\text{BLM/PMC}} (pp \rightarrow t\bar{t}) = 813 \text{ pb}
\]

\[
\sigma_{\text{Conventional}} (pp \rightarrow t\bar{t}) = 794^{+28}_{-39} \text{ pb}
\]

\[
\sigma_{\text{ATLAS}} = 818 \pm 36 \text{ pb}
\]

\[
\sigma_{\text{CMS}} = 803 \pm 32 \text{ pb}
\]
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Impact of ambiguities: Overview

\[ \sigma_{PMC} = s_{2,0} a_s^2(q_2) + s_{3,0} a_s^3(q_3) + s_{4,0} a_s^4(q_4) \]

Table: Total hadronic cross-section through NNLO (in pb)

<table>
<thead>
<tr>
<th></th>
<th>LHC13</th>
<th>Tevatron</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma_{PMC}[q_2, q_3, q_3] )</td>
<td>813</td>
<td>6.48</td>
</tr>
<tr>
<td>( \sigma_{PMC}[q_2, q_3, m_t] )</td>
<td>818</td>
<td>8.30</td>
</tr>
<tr>
<td>( \sigma_{PMC}[q'_2, q'_3, q'_3] )</td>
<td>820</td>
<td>6.97</td>
</tr>
<tr>
<td>( \sigma_{Conventional}[m_t] )</td>
<td>794(^{+28}_{-39})</td>
<td>7.06(^{+0.21}_{-0.25})</td>
</tr>
<tr>
<td>( \sigma_{Experimental} )</td>
<td>818 (\pm) 36 [ATLAS]</td>
<td>7.60 (\pm) 0.41</td>
</tr>
<tr>
<td></td>
<td>803 (\pm) 32 [CMS]</td>
<td></td>
</tr>
</tbody>
</table>
Impact of ambiguities: $q\bar{q}$ channel at LHC

Table: The $q\bar{q}$ channel’s contribution to the LHC13 cross–section for various PMC scale choices.

<table>
<thead>
<tr>
<th>PMC</th>
<th>Conv.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(q_2, q_3, q_3)$</td>
<td>$(q_2, q_3, m_t)$</td>
</tr>
<tr>
<td>$\alpha_s^2$ [pb]</td>
<td>62.4</td>
</tr>
<tr>
<td>$\alpha_s^3$ [pb]</td>
<td>41.7</td>
</tr>
<tr>
<td>$\alpha_s^4$ [pb]</td>
<td>$-32.3$</td>
</tr>
<tr>
<td>NNLO [pb]</td>
<td>71.8</td>
</tr>
</tbody>
</table>

Graphs showing the dependence of PMC scale on $v$ for different choices of $q_2$, $q'_2$, $q_3$, and $q'_3$.
Impact of ambiguities: \( gg \) channel at LHC

**Table:** The \( gg \) channel’s contribution to the LHC13 cross–section for various PMC scale choices.

<table>
<thead>
<tr>
<th>PMC</th>
<th>Conv.</th>
<th>$m_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>( (q_2, q_3, q_3) )</td>
<td>( (q_2, q_3, m_t) )</td>
<td>( (q_2', q_3', q_3') )</td>
</tr>
<tr>
<td>$\alpha_s^2$ [pb]</td>
<td>405.7</td>
<td>405.7</td>
</tr>
<tr>
<td>$\alpha_s^3$ [pb]</td>
<td>256.4</td>
<td>256.4</td>
</tr>
<tr>
<td>$\alpha_s^4$ [pb]</td>
<td>76.4</td>
<td>53.8</td>
</tr>
<tr>
<td>NNLO [pb]</td>
<td>738.4</td>
<td>715.9</td>
</tr>
</tbody>
</table>
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Comparison of strategies to handle the $q_4$ ambiguity

- Most significant ambiguity is choice of highest scale, $q_4$
- PMC requires $N^3 LO$ information to calculate $q_4$
- Can explore possible choices of highest scale by moving to down to NLO, where highest scale is $q_3$
- Recall BLM/PMC at NLO:
  \[ \sigma = s_{2,0} a_s^2 (\mu_R) + [s_{3,0} + 2\beta_0 s_{3,1} (\mu_R)] a_s^3 (\mu_R) \]
  \[ \sigma_{BLM} = s_{2,0} a_s^2 (q_2) + s_{3,0} a_s^3 (q_3) \]
  \[ \log \left( \frac{q_2^2}{\mu_R^2} \right) = -\frac{s_{3,1}(\mu_R)}{s_{2,0}} \]
- Will compare numerical effects of 4 possible choices for $(q_2, q_3)$:
  - $(q_2', q_2')$ \quad \text{NLO information only}
  - $(q_2', m_t)$ \quad \text{NLO information only}
  - $(q_2', q_3')$ \quad “Peeking” at NNLO
  - $(q_2, q_3)$
Choice of $q_3$ at NLO: $q\bar{q}$ channel

\[
\sigma_{BLM/PMC} = s_{2,0}a_s^2(q_2) + s_{3,0}a_s^3(q_3)
\]

**Table:** The $q\bar{q}$ channel’s contribution to the LHC13 cross-section at NLO using various scale choices

<table>
<thead>
<tr>
<th></th>
<th>PMC</th>
<th>Conv.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>($q'_2$, $q'_2$)</td>
<td>($q'_2$, $m_t$)</td>
</tr>
<tr>
<td>$\alpha_s^2$ [pb]</td>
<td>65.1</td>
<td>65.1</td>
</tr>
<tr>
<td>$\alpha_s^3$ [pb]</td>
<td>11.2</td>
<td>12.2</td>
</tr>
<tr>
<td>NLO [pb]</td>
<td>76.3</td>
<td>77.2</td>
</tr>
</tbody>
</table>
Choice of $q_3$ at NLO: $gg$ channel

$$\sigma_{BLM/PMC} = s_{2,0} a_s^2(q_2) + s_{3,0} a_s^3(q_3)$$

Table: The $gg$ channel’s contribution to the LHC13 cross-section at NLO using various scale choices

<table>
<thead>
<tr>
<th>Scale</th>
<th>$\alpha_s^2$ [pb]</th>
<th>$\alpha_s^3$ [pb]</th>
<th>NLO [pb]</th>
<th>Conv. $m_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(q'_2, q'_2)$</td>
<td>405.4</td>
<td>221.3</td>
<td>626.7</td>
<td>406.9</td>
</tr>
<tr>
<td>$(q'_2, m_t)$</td>
<td>405.4</td>
<td>222.3</td>
<td>627.7</td>
<td>220.8</td>
</tr>
<tr>
<td>$(q'_2, q'_3)$</td>
<td>405.4</td>
<td>256.7</td>
<td>662.1</td>
<td></td>
</tr>
<tr>
<td>$(q_2, q_3)$</td>
<td>405.7</td>
<td>256.4</td>
<td>662.1</td>
<td>$67.6_{-63.6}$</td>
</tr>
</tbody>
</table>

$\alpha_s^2$ and $\alpha_s^3$ are the strong coupling constants, $m_t$ is the top quark mass, and $s_{2,0}$ and $s_{3,0}$ are scale choices.
Results
Comparison of strategies to handle the $q_4$ ambiguity

Choice of $q_3$ at NLO: Summary

$$\sigma_{BLM/PMC} = s_{2,0} a_s^2(q_2) + s_{3,0} a_s^3(q_3)$$

**Table:** Total hadronic cross-section through NLO.

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<thead>
<tr>
<th></th>
<th>LHC13</th>
<th>Tevatron</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{PMC}[q'_2, q'_2]$</td>
<td>709</td>
<td>6.52</td>
</tr>
<tr>
<td>$\sigma_{PMC}[q'_2, m_t]$</td>
<td>711</td>
<td>6.51</td>
</tr>
<tr>
<td>$\sigma_{PMC}[q'_2, q'_3]$</td>
<td>762</td>
<td>7.86</td>
</tr>
<tr>
<td>$\sigma_{PMC}[q_2, q_3]$</td>
<td>773</td>
<td>8.59</td>
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<tr>
<td>$\sigma_{Conventional}[m_t]$</td>
<td>$711^{+71}_{-69}$</td>
<td>$6.51^{+0.30}_{-0.44}$</td>
</tr>
<tr>
<td>$\sigma_{Experimental}$</td>
<td>$818 \pm 36$ [ATLAS]</td>
<td>$7.60 \pm 0.41$</td>
</tr>
<tr>
<td></td>
<td>$803 \pm 32$ [CMS]</td>
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</tr>
</tbody>
</table>
Outline

1. Introduction

2. BLM/PMC procedure and $t\bar{t}$ production
   - Introduction to the BLM/PMC procedure
   - Ambiguities in the BLM/PMC procedure
   - $t\bar{t}$ production at NNLO

3. Results
   - PMC scales
   - Hadronic cross-sections at Tevatron and at LHC
   - Impact of ambiguities
   - Comparison of strategies to handle the $q_4$ ambiguity

4. Conclusion
Conclusion

- Identified 3 ambiguities in the PMC procedure. Numerical impact can be significant.

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<tr>
<td>$\sigma_{PMC}[q_2, q_3, q_3]$</td>
<td>813</td>
<td>6.48</td>
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<tr>
<td>$\sigma_{PMC}[q_2, q_3, m_t]$</td>
<td>818</td>
<td>8.30</td>
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<tr>
<td>$\sigma_{PMC}[q'_2, q'_3, q'_3]$</td>
<td>820</td>
<td>6.97</td>
</tr>
<tr>
<td>$\sigma_{Conventional}[m_t]$</td>
<td>$794^{+28}_{-39}$</td>
<td>$7.06^{+0.21}_{-0.25}$</td>
</tr>
<tr>
<td>$\sigma_{Experimental}$</td>
<td>818 ± 36 [ATLAS]</td>
<td>7.60 ± 0.41</td>
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<td>803 ± 32 [CMS]</td>
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</tr>
</tbody>
</table>

- Two known “solutions” for $q_4$ ambiguity. Results differ markedly.
- Full details in arXiv:1907.06610