Determination of the strong coupling beyond NNLO

Gábor Somogyi
Wigner Research Centre for Physics

ELTE particle physics seminar, 5 October 2021
Introduction
The strong coupling $\alpha_s$ is a fundamental parameter of the Standard Model, its value (at a given energy scale) is a basic constant of Nature.

The numerical value of the strong coupling enters essentially all theoretical predictions for LHC processes $\Rightarrow$ the accurate knowledge of this numerical value is important for fully exploiting LHC results.

It is the least precisely known coupling: $\Delta \alpha_s(M_Z)/\alpha_s(M_Z) \sim 1\%$.

<table>
<thead>
<tr>
<th>Coupling</th>
<th>Symbol</th>
<th>Value</th>
<th>Error (ppb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>fine-structure constant</td>
<td>$\alpha_{EM}$</td>
<td>$7.2973525693(11) \times 10^{-3}$</td>
<td>0.15</td>
</tr>
<tr>
<td>Fermi constant</td>
<td>$G_F$</td>
<td>$1.1663787(6) \times 10^{-5}$ GeV$^{-2}$</td>
<td>510</td>
</tr>
<tr>
<td>strong coupling</td>
<td>$\alpha_s(M_Z)$</td>
<td>0.1179(10)</td>
<td>$8.5 \times 10^6$</td>
</tr>
<tr>
<td>gravitational constant</td>
<td>$G_N$</td>
<td>$6.67430(15) \times 10^{-11}$ m$^3$ kg$^{-1}$ s$^{-2}$</td>
<td>$2.2 \times 10^4$</td>
</tr>
</tbody>
</table>

Its value must be extracted by fitting theoretical predictions to measured data $\Rightarrow$ many options depending on the nature of the observable.
The strong coupling: relevance at LHC

The uncertainty in $\alpha_s$ contributes significantly to many QCD predictions, e.g., cross sections for top quark or Higgs boson production.

Consider $pp \rightarrow t\bar{t}$:

- The total cross section $\sigma_{t\bar{t}}$ has been measured:
  \[ \sigma_{t\bar{t}} = 803 \pm 2\text{(stat)} \pm 25\text{(syst)} \pm 20\text{(lumi)} \text{ pb} \]
  
  [CMS Collaboration, EPJC 79 (2019) 5, 368]

- The combined uncertainty corresponds to: $\Delta\sigma_{t\bar{t}}/\sigma_{t\bar{t}} \sim 4\%$

- But $t\bar{t}$ production is proportional to $\alpha_s^2$ already at tree level: $\sigma_{t\bar{t}} \propto \alpha_s^2$

- So at a basic level: $\Delta\sigma_{t\bar{t}}/\sigma_{t\bar{t}} \propto 2\Delta\alpha_s/\alpha_s \sim 2\%$, which is commensurate with the experimental error!
The strong coupling: relevance at LHC

The uncertainty in $\alpha_s$ contributes significantly to many QCD predictions, e.g., cross sections for top quark or Higgs boson production.

Consider $pp \rightarrow t\bar{t} + N$ jets:

- CMS has measured normalized triple differential cross sections in $N_{\text{jet}}$, $M(t\bar{t})$ and $y(t\bar{t})$
  [CMS Collaboration, EPJC 80 (2020) 7, 658]
- For bins with the highest precision, i.e., $N_{\text{jet}} = 0$ and $440 < M(t\bar{t}) < 1500$ GeV, they find uncertainties of around 2–3% (stat.) and 3–6% (syst.)
- Total th. uncertainty: $\sim 7\%$, uncertainty from $\alpha_s$: $\sim 4\%$.
- In many bins, the dominant theoretical uncertainty comes from $\alpha_s$ variation.
The strong coupling: status

### Different approaches

- Many types of observables used to extract the strong coupling over a large energy range of $\sim 1$ GeV ($\tau$ decays) to $\sim 1000$ GeV (LHC inclusive jets)
- By convention and to facilitate comparison, measurements evolved to $Q = M_Z$, plethora of measurements also checks the predicted running

![Graph showing the strong coupling in different energy ranges](image)

[Details of the graph and values provided in the text]

P. A. Zyla et al. (Particle Data Group), Prog. Theor. Exp. Phys. 2020, 083C01 (2020) and 2021 update
The strong coupling from $e^+e^-$ annihilation

Why $\alpha_s$ in $e^+e^-$?

- Electron-positron collisions offer a clean environment for the analysis
- The $e^+e^-$ jets & shapes sub-field alone gives $\sim 2.6\%$ uncertainty due to the large spread between measurements
- Can $\sim 1\%$ precision be achieved?

Why the differences?

- **Hadronization modeling**: Monte Carlo or analytic
- Perturbative order: fixed order NNLO to $N^3$LO + resummation NLL to $N^3$LL
- Type of observable used: jet rates or event shapes

How best to improve?

---

[P. A. Zyla et al. (Particle Data Group), Prog. Theor. Exp. Phys. 2020, 083C01 (2020) and 2021 update]
The strong coupling from $e^+e^-$ annihilation: issues

The current situation raises some questions:

- No new data foreseen in the near future, so would including more perturbative orders (fixed order and/or resummation) improve precision without any new data?
- If not, what are the limiting factors for precision in future QCD studies?
- What should be done to eliminate those factors?

To address these issues, two state-of-the-art pQCD analyses are presented:

1. An analysis based on the two-jet rate $R_2$ computed at $N^3$LO+NNLL accuracy. In this analysis Monte Carlo tools are used to obtain hadronization corrections.


2. An analysis of event shape averages where unknown perturbative corrections beyond NNLO are estimated from data. Hadronization corrections are obtained using both Monte Carlo tools as well as analytic models.

The strong coupling from jet rates
QCD predicts that the hadrons created in electron-positron annihilation are produced in beams of collimated particles – jets.

**Jet finding algorithms** are used to define precisely how many jets are present in an event and which particle belongs to a given jet.

**Durham algorithm** used in this study. Define a “distance measure” on final-state objects

\[
y_{ij} = 2 \frac{\min(E_i^2, E_j^2)}{E_{\text{vis}}^2} (1 - \cos \theta_{ij})
\]

Jets are defined by the following **recursive algorithm**

1. Find the smallest \(y_{ij}\), suppose this is \(\min(y_{ij}) = y_{kl}\).
2. If \(y_{kl}\) is greater than a pre-determined cutoff \(y_{\text{cut}}\) (i.e., \(\min(y_{ij}) > y_{\text{cut}}\)), then we are done, each final-state object is a jet.
3. If \(y_{kl} < y_{\text{cut}}\), then replace the \(k\)-th and \(l\)-th object by a single new object of momentum \(p_k^{\mu} + p_l^{\mu}\).
Jet rates in electron-positron annihilation

**Jet rates:** $R_n$ is the fraction of $n$-jet events for a given $y_{\text{cut}}$

$$R_n(y_{\text{cut}}) = \frac{\sigma_{n\text{-jet}}(y_{\text{cut}})}{\sigma_{\text{tot}}}$$

General behavior easy to understand

- if $y_{\text{cut}}$ is large, there are many steps of combining objects $\Rightarrow$ few jets
- if $y_{\text{cut}}$ is small, there are few steps of combining objects $\Rightarrow$ many jets
- $\sum_n R_n = 1$

Good candidate for $\alpha_s$ measurement

- High perturbative accuracy, especially for $R_2$
- Lots of precise data from LEP (and PETRA)
- Jet rates are known to be less sensitive to hadronization corrections than event shapes
- $R_3$ was used multiple times in the past to extract $\alpha_s(M_Z)$

Jet rates analysis: components

- Data from LEP and PETRA + new OPAL measurements used to build correlation model for older measurements.
- Fixed-order perturbative predictions + some $b$-quark mass corrections
- Resummation + matching
- Non-perturbative corrections from state-of-the-art MC event generators + Lund and cluster hadronization models
Combined analysis using 20+ datasets from 4 collaborations

The data covers a **wide range of CMS energies**: $\sqrt{s} = 35 - 207$ GeV

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Data $\sqrt{s}$, (average), GeV</th>
<th>MC $\sqrt{s}$, GeV</th>
<th>Events</th>
</tr>
</thead>
<tbody>
<tr>
<td>OPAL</td>
<td>91.2(91.2)</td>
<td>91.2</td>
<td>1508031</td>
</tr>
<tr>
<td>OPAL</td>
<td>189.0(189.0)</td>
<td>189</td>
<td>3300</td>
</tr>
<tr>
<td>OPAL</td>
<td>183.0(183.0)</td>
<td>183</td>
<td>1082</td>
</tr>
<tr>
<td>OPAL</td>
<td>172.0(172.0)</td>
<td>172</td>
<td>224</td>
</tr>
<tr>
<td>OPAL</td>
<td>161.0(161.0)</td>
<td>161</td>
<td>281</td>
</tr>
<tr>
<td>OPAL</td>
<td>130.0 – 136.0(133.0)</td>
<td>133</td>
<td>630</td>
</tr>
<tr>
<td>L3</td>
<td>201.5 – 209.1(206.2)</td>
<td>206</td>
<td>4146</td>
</tr>
<tr>
<td>L3</td>
<td>199.2 – 203.8(200.2)</td>
<td>200</td>
<td>2456</td>
</tr>
<tr>
<td>L3</td>
<td>191.4 – 196.0(194.4)</td>
<td>194</td>
<td>2403</td>
</tr>
<tr>
<td>L3</td>
<td>188.4 – 189.9(188.6)</td>
<td>189</td>
<td>4479</td>
</tr>
<tr>
<td>L3</td>
<td>180.8 – 184.2(182.8)</td>
<td>183</td>
<td>1500</td>
</tr>
<tr>
<td>L3</td>
<td>161.2 – 164.7(161.3)</td>
<td>161</td>
<td>424</td>
</tr>
<tr>
<td>L3</td>
<td>135.9 – 140.1(136.1)</td>
<td>136</td>
<td>414</td>
</tr>
<tr>
<td>L3</td>
<td>129.9 – 130.4(130.1)</td>
<td>130</td>
<td>556</td>
</tr>
<tr>
<td>JADE</td>
<td>43.4 – 44.3(43.7)</td>
<td>44</td>
<td>4110</td>
</tr>
<tr>
<td>JADE</td>
<td>34.5 – 35.5(34.9)</td>
<td>35</td>
<td>29514</td>
</tr>
<tr>
<td>ALEPH</td>
<td>91.2(91.2)</td>
<td>91.2</td>
<td>3600000</td>
</tr>
<tr>
<td>ALEPH</td>
<td>206.0(206.0)</td>
<td>206</td>
<td>3578</td>
</tr>
<tr>
<td>ALEPH</td>
<td>189.0(189.0)</td>
<td>189</td>
<td>3578</td>
</tr>
<tr>
<td>ALEPH</td>
<td>183.0(183.0)</td>
<td>183</td>
<td>1319</td>
</tr>
<tr>
<td>ALEPH</td>
<td>172.0(172.0)</td>
<td>172</td>
<td>257</td>
</tr>
<tr>
<td>ALEPH</td>
<td>161.0(161.0)</td>
<td>161</td>
<td>319</td>
</tr>
<tr>
<td>ALEPH</td>
<td>133.0(133.0)</td>
<td>133</td>
<td>806</td>
</tr>
</tbody>
</table>

Data selection:

- measurements with both charged and neutral final state particles
- corrected for detector effects
- corrected for QED initial state radiation
- no overlap with other samples
- sufficient precision
- sufficient information on dataset available
Fixed-order predictions for jet rates

Fixed-order predictions up to and including $\alpha_s^3$ corrections known for some time


$$R_n(y) = \delta_{2,n} + \frac{\alpha_s(Q)}{2\pi} A_n(y) + \left(\frac{\alpha_s(Q)}{2\pi}\right)^2 B_n(y) + \left(\frac{\alpha_s(Q)}{2\pi}\right)^3 C_n(y) + \mathcal{O}(\alpha_s^4)$$

- $R_3$ computed at NNLO accuracy using CoLoRFuINNLO $\Rightarrow$ obtain $R_2$ at $N^3$LO
- very good numerical precision and stability
- $b$-mass corrections from Zbb4: note only NLO for $R_3 \Rightarrow$ NNLO for $R_2$
- mass effects included at distribution level, e.g.
  $$R_2(y) = (1 - r_b)R_2^{N^3LO}(y)_{m_b=0} + r_b R_2^{NNLO}(y)_{m_b\neq0}$$
  where $r_b$ is the fraction of $b$-quark events
  $$r_b = \frac{\sigma_{m_b\neq0}(e^+e^- \rightarrow b\bar{b})}{\sigma_{m_b\neq0}(e^+e^- \rightarrow \text{hardons})}$$
Resummation

Fixed order **diverges** in the limit of \( y \to 0 \) as \( \sim \alpha_s^n \ln^{2n-1} y \), i.e., the fixed-order coefficients at \( n \)-th order include terms \( \{\ln^k y\}_{k=1}^{2n-1} \).

For small \( y \) the logarithms become large, \( \alpha_s^n \ln^{2n-1} y \sim 1 \), invalidating the use of fixed-order perturbation theory.

Logarithmically enhanced terms must be resummed to all orders to obtain a description appropriate in the \( y \to 0 \) limit. Resummation can be systematically improved by resumming more towers of logs: leading logs (LL), next-to-leading logs (NLL), etc.

\[
R_2(y) \sim \left\{\begin{array}{c}
1 \\
+ \alpha_s \left[ \log y + 1 \right] \\
+ \alpha_s^2 \left[ \log^3 y + \log^2 y + \log y + 1 \right] \\
+ \alpha_s^3 \left[ \log^5 y + \log^4 y + \log^3 y + \log^2 y + \cdots \right] \end{array}\right\} \\
\text{LL, NLL, NNLL, N^3LO}
\]
Combining fixed-order and resummed predictions

Fixed-order and resummed calculations are \textit{complementary} to each other: they describe data over different kinematical ranges.

In order to obtain predictions over a wide kinematical range, the two computations must be \textit{combined} without double counting ("matching").

Matched predictions at $N^3\text{LO}+\text{NNLL}$:

- all terms from first four rows ($N^3\text{LO}$)
- in addition, first three terms from all rows (NNLL)
- must take care to count the first three terms of the first four rows only once

$$R_2(y) \sim \left\{ \begin{array}{c}
1 \\
+ \alpha_s \left[ \log y + 1 \right] \\
+ \alpha_s^2 \left[ \log^3 y + \log^2 y + \log y + 1 \right] \\
+ \alpha_s^3 \left[ \log^5 y + \log^4 y + \log^3 y + \log^2 y + \ldots \right] \end{array} \right\}$$

\text{LO} \quad \text{NLO} \quad \text{NNLO} \quad \text{N}^3\text{LO}
Resummed predictions for jet rates

Resummed predictions for $R_2$ at **NNLL** accuracy have been computed more recently


$$R_2(y) = e^{-R_{NNLL}(y)} \left[ \left( 1 + \frac{\alpha_s(Q)}{2\pi} H^{(1)} + \frac{\alpha_s(Q\sqrt{y})}{2\pi} C_{hc}^{(1)} \right) F_{NLL}(y) + \frac{\alpha_s(Q)}{2\pi} \delta F_{NNLL}(y) \right]$$

- resummation performed with the ARES program
- matching to fixed-order: log $R$ scheme
- counting of logs (NNLL) here refers to logs in $\ln R_2$

In contrast, resummed predictions for $R_3$ have a much lower logarithmic accuracy

- more colored emitters
- state-of-the-art resummation includes only $O(\alpha^n_s L^{2n})$ and $O(\alpha^n_s L^{2n-1})$ terms in $R_3$
  (note different logarithmic counting)
- in this analysis, no resummation for $R_3$ is performed

↓

**Main focus on N$^3$LO+NNLL for $R_2$, but also simultaneous analysis with NNLO for $R_3$**
Hadronization corrections: setups

Effects associated with the parton-to-hadron transition cannot be computed in perturbation theory and must be estimated by other means.

In this analysis: obtained using state-of-the-art MC event generators: $e^+e^- \rightarrow jjjjj$ merged samples with massive $b$-quarks

- Default setup “$H^L$”: Herwig7.1.4 for $e^+e^- \rightarrow 2, 3, 4, 5$ jets, 2 and 3 jets at NLO using MadGraph5 and OpenLoops + Lund fragmentation model
- Setup for hadronization systematics “$H^C$”: Herwig7.1.4 for $e^+e^- \rightarrow 2, 3, 4, 5$ jets, 2 and 3 jets at NLO using MadGraph5 and OpenLoops + cluster fragmentation model
- Setup for cross-checks “$S^C$”: Sherpa2.2.6 for $e^+e^- \rightarrow 2, 3, 4, 5$ jets, 2 jets at NLO using AMEGIC, COMIX and OpenLoops + cluster fragmentation model
Hadronization correction factors

Hadronization correction factors for several values of $y_{\text{cut}}$ for $R_2$ and $R_3$

- Correlations between $R_2$ and $R_3$ taken into account.
- Simultaneous corrections for $R_2$ and $R_3$ preserve physical constraints

$$R_{n,\text{hadrons}} \geq 0, \quad R_{2,\text{hadrons}} + R_{3,\text{hadrons}} + R_{\geq 4,\text{hadrons}} = 1$$
Fit procedure

To find the optimal value of $\alpha_s$, MINUIT2 is used to minimize

$$\chi^2(\alpha_s) = \sum_{\text{data set}} \chi^2(\alpha_s)_{\text{data set}}$$

where $\chi^2(\alpha_s)$ are computed separately for each data set

$$\chi^2(\alpha_s) = \vec{r} V^{-1} \vec{r}^T, \quad \vec{r} = (\vec{D} - \vec{P}(\alpha_s))$$

- $\vec{D}$: vector of data points
- $\vec{P}(\alpha_s)$: vector of theoretical predictions
- $V$: covariance matrix for $\vec{D}$ (statistical correlations estimated from MC generated samples, systematic correlations modeled to mimic patterns observed in OPAL data)
Central result and fit range selection

- avoid regions where theoretical predictions or hadronization model are unreliable
- $Q^2$-dependent fit range: $[-2.25 + \mathcal{L}, -1]$ for $R_2$ and $[-2 + \mathcal{L}, -1]$ for $R_3$ (if used), where $\mathcal{L} = \ln \frac{M_N^2}{Q^2}$
- note separate fit ranges for $R_2$ and $R_3$ (if used)
- smallest $\chi^2 / ndof$, low sensitivity to fit range
Estimate the uncertainty by

- varying the renormalization scale
  $\mu_{\text{ren}} \in [Q/2, 2Q]$:
  \( (\text{ren}) \)

- varying the resummation scale
  $\mu_{\text{res}} \in [Q/2, 2Q]$:
  \( (\text{res}) \)

- varying the hadronization model
  $H^L$ vs. $H^C$:
  \( (\text{hadr}) \)

- fit uncertainty is obtained from the
  $\chi^2 + 1$ criterion as implemented in MINUIT2:
  \( (\text{exp}) \)

Notice much reduced renormalization scale uncertainty when NNLL resummation for $R_2$ is included.
Results: $R_2$

Extraction of $\alpha_s(M_Z)$ from the two-jet rate $R_2$ measured over a wide range of cms energies in $e^+e^-$ collisions has been performed at N$^3$LO+NNLL accuracy for the first time:

$$\alpha_s(M_Z) = 0.11881 \pm 0.00063(\text{exp.}) \pm 0.00101(\text{hadr.}) \pm 0.00045(\text{ren.}) \pm 0.00034(\text{res.})$$

$$\alpha_s(M_Z) = 0.11881 \pm 0.00131(\text{comb.})$$

- main source of uncertainty: **hadronization modeling**
- uncertainty from scale variation is considerably smaller than from hadronization
- experimental uncertainty comparable to perturbative one

Inclusion of **NNLL resummation crucial** for reducing perturbative uncertainty
Combined fit of $R_2$ at N$^3$LO+NNLL and $R_3$ at NNLO, taking into account for the first time the correlation between the observables gives:

$$\alpha_s(M_Z) = 0.11989 \pm 0.00045(\text{exp.}) \pm 0.00098(\text{hadr.}) \pm 0.00046(\text{ren.}) \pm 0.00017(\text{res.})$$

$$\alpha_s(M_Z) = 0.11989 \pm 0.00118(\text{comb.})$$

- result is fully compatible with $R_2$-only fit
- formally more precise than a fit based on $R_2$ alone,
- but much more sensitive to fit range selection

An accurate resummation of $R_3$ could potentially reduce the sensitivity to fit range selection and lead to an even more precise determination of $\alpha_s(M_Z)$
The strong coupling from jet rates: final result

The following value of $\alpha_s(M_Z)$ was obtained in the analysis

$$\alpha_s(M_Z) = 0.11881 \pm 0.00063 \, (exp.) \pm 0.00101 \, (hadr.) \pm 0.00045 \, (ren.) \pm 0.00034 \, (res.)$$

$$\alpha_s(M_Z) = 0.11881 \pm 0.00131 \, (comb.)$$

- The result agrees with the world average $\alpha_s(M_Z)_{PDG2020} = 0.1179 \pm 0.0010$ and has an uncertainty that is of the same size
- The presented result is the most precise in its subclass [Salam, arXiv:1712.05165v2]

<table>
<thead>
<tr>
<th>Determination</th>
<th>Data and procedure</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1175 ± 0.0025</td>
<td>ALEPH 3-jet rate (NNLO+MChad)</td>
</tr>
<tr>
<td>0.1199 ± 0.0059</td>
<td>JADE 3-jet rate (NNLO+NLL+MChad)</td>
</tr>
<tr>
<td>0.1224 ± 0.0039</td>
<td>ALEPH event shapes (NNLO+NLL+MChad)</td>
</tr>
<tr>
<td>0.1172 ± 0.0051</td>
<td>JADE event shapes (NNLO+NLL+MChad)</td>
</tr>
<tr>
<td>0.1189 ± 0.0041</td>
<td>OPAL event shapes (NNLO+NLL+MChad)</td>
</tr>
<tr>
<td>0.1164^{+0.0028}_{-0.0026}</td>
<td>Thrust (NNLO+NLL+anlhad)</td>
</tr>
<tr>
<td>0.1134^{+0.0031}_{-0.0025}</td>
<td>Thrust (NNLO+NNLL+anlhad)</td>
</tr>
<tr>
<td>0.1135 ± 0.0011</td>
<td>Thrust (SCET NNLO+N^3LL+anlhad)</td>
</tr>
<tr>
<td>0.1123 ± 0.0015</td>
<td>C-parameter (SCET NNLO+N^3LL+anlhad)</td>
</tr>
</tbody>
</table>
So what is the issue?

The main source of uncertainty is due to hadronization modeling and differences with other precise determinations remain.

Monte Carlo simulations used to obtain hadronization corrections, but

- the parton level of the MC simulation is not equivalent to a fixed-order calculation
- the tuning of the shower/hadronization models performed using theoretical predictions with lower perturbative accuracy

Sizeable difference with other precise determinations, e.g. those based on thrust ($T$). Basic differences

- NNLO vs. $N^3$LO perturbative accuracy
- Monte Calo vs. analytic hadronization models

Can we examine the role of higher orders and hadronization models in a single analysis?
The strong coupling from event shape averages
To address this question, we perform a state-of-the-art perturbative QCD analysis of event shape averages.

**Event shapes** associate a single number to the entire event, describing some specific aspect of the global event topology.

**Thrust (T):**

- Definition: \( T = \max_{\vec{n}} \left( \frac{\sum_i |\vec{n} \cdot \vec{p}_i|}{\sum_i |\vec{p}_i|} \right) \)

- Generally \( 1/2 \leq T \leq 1 \), where \( T = 1/2 \) for spherically symmetric events and \( T \to 1 \) in the dijet limit ("pencil-like" event)
To address this question, we perform a state-of-the-art perturbative QCD analysis of event shape averages.

**Event shapes** associate a single number to the entire event, describing some specific aspect of the global event topology.

**C-parameter** ($C$):

- **Definition**: $C = 3(\lambda_1 \lambda_2 + \lambda_2 \lambda_3 + \lambda_3 \lambda_1)$, $\lambda_i$ are eigenvalues of $\Theta^{\rho\sigma} = \frac{1}{\sum_i |\vec{p}_i|} \sum_i \frac{\vec{p}_i^\rho \vec{p}_i^\sigma}{|\vec{p}_i|}$

- Generally $0 \leq C \leq 1$, where $C = 1$ for spherically symmetric events and $C \to 0$ in the dijet limit (“pencil-like” event). For planar events $0 \leq C \leq 3/4$. 

![Diagram: Event shapes](image)
Event shapes

Three-jet event shapes (i.e., those that have a non-trivial distribution already with three final-state momenta) can be computed to **NNLO** accuracy in pQCD (note $\tau = 1 - T$).


Clearly **event shape moments** can also be computed at the same accuracy.
• Data form 20+ datasets with a wide range of energies: focus on thrust ($T$) and the $C$-parameter ($C$).

• Estimation of unknown $N^3$LO perturbative QCD coefficients from data (hence the focus on event shape averages $\Rightarrow$ small number of coefficients to fit).

• Hadronization corrections obtained from both Monte Carlo tools as well as analytic models extended to $N^3$LO for the first time.
**Combined analysis** using 20+ datasets and a **wide range of energies**: $\sqrt{s} = 29–206$ GeV

<table>
<thead>
<tr>
<th>Source</th>
<th>Measured Observables</th>
<th>Measured $\sqrt{s}$ range (GeV)</th>
<th>Used Observables</th>
<th>Used $\sqrt{s}$ range (GeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALEPH</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[133]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[133]</td>
</tr>
<tr>
<td>ALEPH</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[91]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[91]</td>
</tr>
<tr>
<td>ALEPH</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>9,[91, 206]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>9,[91, 206]</td>
</tr>
<tr>
<td>AMY</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[55]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[55]</td>
</tr>
<tr>
<td>DELPHI</td>
<td>$\langle (1 - T)^{1,2,3} \rangle$</td>
<td>15,[91, 183]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>5,[91, 183]</td>
</tr>
<tr>
<td>DELPHI</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>15,[45, 202]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>11,[45, 202]</td>
</tr>
<tr>
<td>HRS</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[29]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[29]</td>
</tr>
<tr>
<td>JADE</td>
<td>$\langle (1 - T)^{1,2,3,4,5} \rangle$</td>
<td>30,[14, 43]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>4,[34, 43]</td>
</tr>
<tr>
<td>L3</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[91]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[91]</td>
</tr>
<tr>
<td>L3</td>
<td>$\langle (1 - T)^{1,2} \rangle$</td>
<td>30,[41, 206]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>15,[41, 206]</td>
</tr>
<tr>
<td>MARK</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[89]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[89]</td>
</tr>
<tr>
<td>MARK</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[29]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[29]</td>
</tr>
<tr>
<td>MARKII</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[89]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>1,[89]</td>
</tr>
<tr>
<td>OPAL</td>
<td>$\langle (1 - T)^{1,2,3,4,5} \rangle$</td>
<td>60,[91, 206]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>12,[91, 206]</td>
</tr>
<tr>
<td>TASSO</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>4,[14, 44]</td>
<td>$\langle (1 - T)^1 \rangle$</td>
<td>2,[35, 44]</td>
</tr>
<tr>
<td>ALEPH</td>
<td>$\langle C^1 \rangle$</td>
<td>1,[91]</td>
<td>$\langle C^1 \rangle$</td>
<td>1,[91]</td>
</tr>
<tr>
<td>DELPHI</td>
<td>$\langle C^1 \rangle$</td>
<td>15,[45, 202]</td>
<td>$\langle C^1 \rangle$</td>
<td>11,[45, 202]</td>
</tr>
<tr>
<td>DELPHI</td>
<td>$\langle C^{1,2,3} \rangle$</td>
<td>12,[133, 183]</td>
<td>$\langle C^1 \rangle$</td>
<td>4,[133, 183]</td>
</tr>
<tr>
<td>JADE</td>
<td>$\langle C^{1,2,3,4,5} \rangle$</td>
<td>30,[14, 43]</td>
<td>$\langle C^1 \rangle$</td>
<td>4,[34, 43]</td>
</tr>
<tr>
<td>L3</td>
<td>$\langle C^1 \rangle$</td>
<td>1,[91]</td>
<td>$\langle C^1 \rangle$</td>
<td>1,[91]</td>
</tr>
<tr>
<td>L3</td>
<td>$\langle C^{1,2} \rangle$</td>
<td>18,[130, 206]</td>
<td>$\langle C^1 \rangle$</td>
<td>9,[130, 206]</td>
</tr>
<tr>
<td>OPAL</td>
<td>$\langle C^{1,2,3,4,5} \rangle$</td>
<td>60,[91, 206]</td>
<td>$\langle C^1 \rangle$</td>
<td>12,[91, 206]</td>
</tr>
</tbody>
</table>
Fixed-order predictions for event shape moments

The $n$-th moment of an event shape $O$ is defined by

$$\langle O^n \rangle = \frac{1}{\sigma_{\text{tot}}} \int_{O_{\text{min}}}^{O_{\text{max}}} O^n \frac{d\sigma(O)}{dO} dO$$

Fixed-order predictions up to and including $\alpha_s^4$ terms read

$$\langle O^n \rangle = \frac{\alpha_s(Q)}{2\pi} A^{O^n} + \left( \frac{\alpha_s(Q)}{2\pi} \right)^2 B^{O^n} + \left( \frac{\alpha_s(Q)}{2\pi} \right)^3 C^{O^n} + \left( \frac{\alpha_s(Q)}{2\pi} \right)^4 D^{O^n} + \mathcal{O}(\alpha_s^5)$$

- First three coefficients ($A^{O^n}$, $B^{O^n}$ and $C^{O^n}$) have been known for some time
- Recomputed for this study with CoLoR FuNNLO $\Rightarrow$ very good numerical precision
- $b$-mass corrections from Zbb4: note only NLO

$$A^{O^n} = (1 - r_b(Q)) A_{m_b=0}^{O^n} + r_b(Q) A_{m_b \neq 0}^{O^n}$$

$$B^{O^n} = (1 - r_b(Q)) B_{m_b=0}^{O^n} + r_b(Q) B_{m_b \neq 0}^{O^n}$$

where $r_b$ is the fraction of $b$-quark events

$$r_b(Q) = \frac{\sigma_{m_b \neq 0}(e^+ e^- \rightarrow b\bar{b})}{\sigma_{m_b \neq 0}(e^+ e^- \rightarrow \text{hadrons})}$$
Event shape averages: predictions at NNLO and beyond

We focus on averages of the $C$-parameter $\langle C^1 \rangle$ and one minus thrust $\langle (1 - T)^1 \rangle$

- abundance of available measurements (see above)
- avoid correlations between various moments (not reported by most measurements)

Fixed-order predictions at scale $Q = m_Z$ for the perturbative coefficients [normalized to the leading order cross section $\sigma_0(e^+e^- \rightarrow \text{hadrons})$]

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>This work</th>
<th>Analytic</th>
<th>GGGH</th>
<th>SW</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_0^{\langle (1 - T)^1 \rangle}$</td>
<td>2.1034(1)</td>
<td>2.10347</td>
<td>2.1035</td>
<td>2.10344(3)</td>
</tr>
<tr>
<td>$B_0^{\langle (1 - T)^1 \rangle}$</td>
<td>44.995(1)</td>
<td>44.999(2)</td>
<td>867(21)</td>
<td>44.999(5)</td>
</tr>
<tr>
<td>$C_0^{\langle (1 - T)^1 \rangle}$</td>
<td>979.6(6)</td>
<td>867(21)</td>
<td>1100(30)</td>
<td></td>
</tr>
<tr>
<td>$A_0^{\langle C^1 \rangle}$</td>
<td>8.6332(5)</td>
<td>8.63789</td>
<td>8.6379</td>
<td>8.6378(1)</td>
</tr>
<tr>
<td>$B_0^{\langle C^1 \rangle}$</td>
<td>172.834(5)</td>
<td>172.778(7)</td>
<td>172.8(3)</td>
<td>172.8(3)</td>
</tr>
<tr>
<td>$C_0^{\langle C^1 \rangle}$</td>
<td>3525(3)</td>
<td>3212(89)</td>
<td>4200(100)</td>
<td></td>
</tr>
</tbody>
</table>


We extract $D^{\langle (1 - T)^1 \rangle}$ and $D^{\langle C^1 \rangle}$ from data together with $\alpha_s(M_Z)$ in the analysis.
Importantly, the main point of extracting the N$^3$LO coefficients $D\langle(1-T)^1\rangle$ and $D\langle C^1\rangle$ from data is not to get an accurate determination of these quantities.

Rather, it is to model them as best as possible in order to be able to assess the impact of including terms beyond NNLO in the extraction of the strong coupling in the absence of an actual calculation of those terms.
The modeling of non-perturbative corrections is essential to perform a meaningful comparison of predictions with data.

To basic approaches

1. **Monte Carlo (MC) hadronization**: extract hadronization corrections from Monte Carlo simulations.
   
   **Issue**: the parton level of an MC simulation is not equivalent to a fixed-order calculation + issue of tuning.

2. **Analytic hadronization**: use analytic models to describe the effects of hadronization on observables.
   
   **Issue**: systematics are difficult to control.

Apply both approaches and examine the impact of the choice on the extracted value of the strong coupling.
Monte Carlo hadronization

Hadronization corrections obtained using state-of-the-art MC event generators: $e^+e^- \rightarrow Z/\gamma \rightarrow 2, 3, 4, 5$ parton processes generated using MadGraph5 and OpenLoops, 2-parton final state at NLO.

To study hadronization systematics, we employ different setups (similar to jet rates analysis):

- **Default setup “$H^L$”: Herwig7.2.0 with Lund fragmentation model**
- Setup for systematics “$H^C$”: Herwig7.2.0 with cluster fragmentation model
- Setup for cross-checks “$S^C$”: Sherpa2.2.8 with cluster fragmentation model

Hadronization corrections are ratios of observables calculated from MC generated events at hadron and parton levels.

To account for the presence of a shower cut-off scale $Q_0 \approx \mathcal{O}(1 \text{ GeV})$ in MC generators, predictions were computed with several values of $Q_0$ and extrapolated to $Q_0 \rightarrow 0 \text{ GeV}$.

$$
\langle O^n \rangle_{\text{corrected}} = \langle O^n \rangle_{\text{theory}} \times \frac{\langle O^n \rangle_{\text{MC hadrons, } Q_0=0 \text{ GeV}}}{\langle O^n \rangle_{\text{MC partons, } Q_0=0 \text{ GeV}}}
$$
Monte Carlo hadronization

Data and predictions by MC event generators extrapolated to $Q_0 \to 0$ GeV.

- Hadron and parton level MC predictions provide reasonable descriptions of data and NNLO theory for wide range of energy
- Non-physical behaviour of MC parton level results for small $\sqrt{s}$: $\langle O^n \rangle$ increases with energy
Monte Carlo hadronization

Data and predictions by MC event generators extrapolated to $Q_0 \rightarrow 0$ GeV.

- Hadron and parton level MC predictions provide **reasonable descriptions** of data and NNLO theory for wide range of energy
- **Non-physical** behaviour of MC parton level results for small $\sqrt{s}$: $\langle O^n \rangle$ increases with energy

\[
\downarrow
\]

- **Exclude measurements** with $\sqrt{s} < 29$ GeV
- Weaker criterion than requiring that MC matches data well, but retains as much data as possible
Analytic hadronization

**Dispersive model** of analytic hadronization corrections for event shapes: hadronization corrections simply shift the perturbative event shape distributions

\[
\frac{d\sigma_{\text{hadrons}}(O)}{dO} = \frac{d\sigma_{\text{partons}}(O - a_0 P)}{dO}
\]

- the \(a_0\) are observable-specific **constants**, e.g., \(a_{1-T} = 2\) and \(a_C = 3\pi\)
- the power correction \(P\) is **universal**

\[
P(\alpha_s, Q, \alpha_0) = \frac{4C_F}{\pi^2} M \times \frac{\mu_I}{Q} \times \left\{ \alpha_0(\mu_I) - \alpha_S + \mathcal{O}(\alpha_s^2) \right\}
\]

where \(M\) is the so-called Milan factor and \(\alpha_0\) is a non-perturbative model parameter

Under these **assumptions**, we find that non-perturbative corrections simply shift the perturbative event shape averages

\[
\langle O^1 \rangle_{\text{hadrons}} = \langle O^1 \rangle_{\text{partons}} + a_0 P
\]
Issues with the dispersive model

Recently, both of these assumptions have been challenged

- the $a_O$ are observable-specific **constants**

  **Issue:** $a_O$ have been computed in the two-jet limit, but they actually depend on the value of $O$. This dependence is a source of uncertainty in $\alpha_s$ extractions based on event shapes and analytic hadronization models that has not been accounted for so far and may be responsible for some of the tension between recent $\alpha_s$ determinations.


- the power correction $\mathcal{P}$ is **universal**

  \[
  \mathcal{P}(\alpha_s, Q, \alpha_0) = \frac{4C_F}{\pi^2} \mathcal{M} \times \frac{\mu_I}{Q} \times \left\{ \alpha_0(\mu_I) - \alpha_S + \mathcal{O}(\alpha_s^2) \right\}
  \]

  **Issue:** non-inclusive corrections, e.g., those parametrized by the Milan factor $\mathcal{M}$ may not in fact be universal beyond NLO

In this analysis we take the pragmatic viewpoint that this approach nevertheless provides a reasonable model for non-perturbative corrections. However, the applicability of the dispersive model should be investigated.
Computing the power correction

We must compute $\mathcal{P}$ at $\mathcal{O}(\alpha_s^4)$ accuracy. Ingredients of the computation are

- The running of the strong coupling in the $\overline{\text{MS}}$ scheme
- The relation between the effective soft coupling in the Catani–Marchesini–Webber (CMW) scheme $\alpha_{\text{CMW}}$ and the strong coupling defined in the $\overline{\text{MS}}$ scheme $\alpha_s$

\[
\alpha_{\text{CMW}} = \alpha_s \left[ 1 + \frac{\alpha_s}{2\pi} K + \left( \frac{\alpha_s}{2\pi} \right)^2 L + \left( \frac{\alpha_s}{2\pi} \right)^3 M + \mathcal{O}(\alpha_s^4) \right]
\]

- $K$, $L$ and $M$ are in principle computable constants
- $K$ is simply the one-loop cusp anomalous dimension
- $L$ and $M$ can be computed once the effective soft coupling is explicitly defined $\Rightarrow$ several proposals in the literature beyond NLL, so $L$ and $M$ are “scheme-dependent”
Effective soft coupling schemes

The Catani–Marchesini–Webber soft coupling at NLL ($\alpha_s$ is the strong coupling in the MS scheme, $C_q = C_F$, $C_g = C_A$)

$$A_i^{CMW}(\alpha_s) = C_i \frac{\alpha_s^{CMW}}{\pi} = C_i \frac{\alpha_s^{CMW}}{\pi} \left(1 + \frac{\alpha_s}{2\pi} K\right)$$

Proposals for definitions beyond NLL

$$A_{T,i}(\alpha_s) = \frac{1}{2} \mu^2 \int_0^\infty dm_T^2 dk_T^2 \delta(\mu^2 - k_T^2) w_i(k)$$

$$A_{0,i}(\alpha_s) = \frac{1}{2} \mu^2 \int_0^\infty dm_T^2 dk_T^2 \delta(\mu^2 - m_T^2) w_i(k)$$

where $w_i(k)$ is called the web function, it gives the “probability” of correlated emission (including the corresponding virtual corrections) of an arbitrary number of soft partons with total momentum $k$.

Effective soft coupling schemes

Given these definitions, the expansion of $\alpha_s^{CMW}$ in terms of $\alpha_s$, and hence $L$ and $M$, can in principle be computed (note in each scheme $K$ is the one-loop cusp anomalous dimension)

$$(\alpha_s^{CMW})_{\text{scheme}} = \alpha_s \left[ 1 + \frac{\alpha_s}{2\pi} K + \left( \frac{\alpha_s}{2\pi} \right)^2 L_{\text{scheme}} + \left( \frac{\alpha_s}{2\pi} \right)^3 M_{\text{scheme}} + \mathcal{O}(\alpha_s^4) \right]$$

- $A^0$ scheme: $L$ and $M$ computed from $A_{0,i}$
- $A^T$ scheme: $L$ computed from $A_{T,i}$, but the complete expression for $M$ is missing in this scheme, hence we set $M_T = M_0$
- $A^{\text{cusp}}$ scheme: $L$ and $M$ are simply set equal to the two-and three-loop cusp anomalous dimensions (for ease of comparison with existing results)
The power correction

The power correction at $O(\alpha_s^4)$ accuracy reads

$$\mathcal{P}(\alpha_s, Q, \alpha_0) = \frac{4C_F}{\pi^2} \mathcal{M} \times \frac{\mu_I}{Q} \times \left\{ \alpha_0(\mu_I) - \left[ \alpha_S(\mu_R) + \left( K + \beta_0 \left( 1 + \ln \frac{\mu_R}{\mu_I} \right) \right) \frac{\alpha_S^2(\mu_R)}{2\pi} \right. \right.$$

$$+ \left( 2L + (4\beta_0(\beta_0 + K) + \beta_1) \left( 1 + \ln \frac{\mu_R}{\mu_I} \right) \right) \frac{2\beta_0^2 \ln^2 \frac{\mu_R}{\mu_I}}{8\pi^2} \left. \frac{\alpha_S^3(\mu_R)}{2\pi} \right\}$$

$$+ \left( 4M + (2\beta_0(12\beta_0(\beta_0 + K) + 5\beta_1) + \beta_2 + 4\beta_1 K + 12\beta_0 L) \left( 1 + \ln \frac{\mu_R}{\mu_I} \right) \right.$$

$$+ \beta_0(12\beta_0(\beta_0 + K) + 5\beta_1) \ln^2 \frac{\mu_R}{\mu_I} + 4\beta_0^3 \ln^3 \frac{\mu_R}{\mu_I} \left. \frac{\alpha_S^4(\mu_R)}{32\pi^3} \right\} \right\}$$

- $\mathcal{M}$ is the so-called Milan factor with estimated value $M_{\text{est.}} \pm \delta M_{\text{est.}} = 1.49 \pm 0.30$.
- $\mu_I$ is the scale where the perturbative and non-perturbative couplings are matched. Following the usual choice, we set $\mu_I = 2$ GeV.
- $\alpha_0(\mu_I)$ corresponds to the first moment of the effective soft coupling below the scale $\mu_I$ and is a non-perturbative parameter of the model

$$\alpha_0(\mu_I) = \frac{1}{\mu_I} \int_0^{\mu_I} d\mu \alpha_s^{CMW}(\mu)$$
Hadronization correction factors

Ratios of hadron-level to parton-level predictions

- Analytic hadronization: the result for the $A^0$ scheme is shown, but the different schemes give very similar results.
Hadronization correction factors

Ratios of hadron-level to parton-level predictions

- Analytic hadronization: the result for the $A^0$ scheme is shown, but the different schemes give very similar results.
- Recall measurements with $\sqrt{s} < 29$ GeV are excluded.
- Weaker criterion than requiring that sub-leading power corrections are small.
- Serves to highlight the discrepancies between MC and analytic models where hadronization effects are most pronounced (low energies).
Values of $\alpha_s$ determined using optimization procedures in MINUIT2

$$\chi^2(\alpha_s) = \sum_i \chi_i^2(\alpha_s)$$

where $\chi_i^2(\alpha_s)$ for data set $i$ is

$$\chi_i^2(\alpha_s) = (\vec{D} - \vec{P}(\alpha_s))V^{-1}(\vec{D} - \vec{P}(\alpha_s))^T$$

- $\vec{D}$: vector of data points
- $\vec{P}(\alpha_s)$: vector of calculated predictions
- $V$: the covariance matrix of $\vec{D}$ (diagonal, stat. and syst. uncertainties added in quadrature for every measurement)
Results of the fits at N^3LO vs. data. In addition to $\alpha_s(M_Z)$, we fit also

- the $\mathcal{O}(\alpha_s^4)$ perturbative coefficient $D^{\langle O^n \rangle}$ (in N^3LO fits)
- the non-perturbative parameter $\alpha_0(2\text{ GeV})$ (when using the analytic hadronization model)
- the Milan factor $M$, in order to include the uncertainty on its theoretical value consistently (constrained fit)
- since the dependence on analytic hadronization scheme is mild so only the result for the $A^0$ scheme is shown
Results: $\alpha_s(M_Z)$

The extractions of $\alpha_s(M_Z)$ from $\langle(1 - T)^1\rangle$ and $\langle C^1\rangle$ data

- Good agreement between fits to $\langle(1 - T)^1\rangle$ and $\langle C^1\rangle$ data both at NNLO and $N^3LO \Rightarrow$ internal consistency of extraction procedure
- Analytic hadronization scheme-dependence is mild.
- Large discrepancy between results obtained with MC and analytic hadronization models both at NNLO and $N^3LO \Rightarrow$ suggests that the discrepancy has a fundamental origin and would hold even with exact $N^3LO$ predictions.
- Better understanding of hadronization is key.
Results: $D^{(O^n)}$

The extractions of the $O(\alpha_s^4)$ perturbative coefficients $D^{((1-T)^1)}$ and $D^{(C^1)}$ from data

- Extracted values of the perturbative coefficients show reasonable agreement for both observables between fits using MC and analytic hadronization models ⇒ demonstrates the viability of extracting higher-order coefficients from data.
- The amount and consistency of current data is an issue, would need large amounts of consistent data, e.g., from FCC-ee or CEPC.
- Precise high-energy data would be especially valuable.
The extractions of the non-perturbative parameter $\alpha_0(2\text{ GeV})$ from $\langle (1 - T)^1 \rangle$ and $\langle C^1 \rangle$ data

- Recall this parameter is scheme-dependent, so its values in different schemes should not be directly compared. Nevertheless, the choice of scheme has only a small numerical impact.
- Values extracted from $\langle (1 - T)^1 \rangle$ and $\langle C^1 \rangle$ data agree well with each other both at NNLO and N$^3$LO.
- Rather large uncertainties at N$^3$LO primarily due to insufficient amount and quality of data as well as the extraction method itself.
What did we learn?

The aim of the analysis was to examine the role higher order corrections and the choice of hadronization models play in a single analysis.

In particular, we wanted to assess the factors that will determine the precision of QCD analyses of $e^+e^-$ data once theoretical predictions at $O(\alpha_s^4)$ accuracy become available.

To do this, we have performed an extraction of $\alpha_s(M_Z)$ from the averages of event shapes $\langle (1 - T)^1 \rangle$ and $\langle C^1 \rangle$.

- Using **NNLO theory** and **analytic hadronization models**, the obtained results are consistent with the last world average $\alpha_s(M_Z)^{PDG2020} = 0.1179 \pm 0.0010$.

- We considered a method of extracting $\alpha_s(M_Z)$ at $N^3$LO by estimating the missing $O(\alpha_s^4)$ perturbative coefficient from data. The values of $\alpha_s(M_Z)$ obtained in this way are compatible with the last world average, within somewhat large uncertainties, e.g.,

$$\alpha_s(M_Z)^{N^3LO + A^0} = 0.12911 \pm 0.00177(exp.) \pm 0.0123(scale)$$

- Both MC and analytic hadronization models were used, the latter being extended to $O(\alpha_s^4)$ for the first time.

- The comparison of results obtained with MC and analytic hadronization suggests that **future extractions of $\alpha_s(M_Z)$ will be strongly affected by the modeling of hadronization effects**.
Lessons
Improving perturbative predictions

Improving the perturbative predictions is clearly important.

More N’s, more legs

- beyond NNLO for 3-jet rate/event shapes
- beyond 3-jet rate/event shapes at NNLO
  - improved logarithmic accuracy
  - for 3-jet rate/event shapes

Mass effects, mixed EW×QCD corrections

- mass corrections (finite $m_b$) beyond NLO
- mixed EW×QCD corrections
Improving the perturbative predictions is clearly important.

More N’s, more legs

- beyond NNLO for 3-jet rate/event shapes ⇒ ultimate precision, but may be of limited use by itself
- beyond 3-jet rate/event shapes at NNLO ⇒ would be nice. . .
- improved logarithmic accuracy for 3-jet rate/event shapes ⇒ already within reach!

Mass effects, mixed EW×QCD corrections

- mass corrections (finite $m_b$) beyond NLO ⇒ more relevant
- mixed EW×QCD corrections ⇒ more relevant
Improving the perturbative predictions is clearly important.

More N’s, more legs

- beyond NNLO for 3-jet rate/event shapes
- beyond 3-jet rate/event shapes at NNLO
- improved logarithmic accuracy for 3-jet rate/event shapes

Mass effects, mixed EW×QCD corrections

- mass corrections (finite $m_b$) beyond NLO
- mixed EW×QCD corrections

However

- the necessary 2- and 3-loop matrix elements are presently not known, however this is a very active area, so expect new results
- using those matrix elements to compute physical observables is a separate issue in itself (definitely beyond NNLO), new ideas may be needed
The role of hadronization corrections

But the **elephant in the room**: hadronization modeling

- discrepancies between results obtained with MC and analytic hadronization models will likely remain in place even after including exact higher order perturbative corrections beyond NNLO
- naively going to higher energies helps: hadr. corr. $\sim 1/Q$, however…
- the energy of foreseen machines (FCC-ee, CEPC) is not orders of magnitude larger than LEP
- moreover, going up in energy there is non-trivial interplay between smaller hadronization corrections but larger background and much smaller luminosity
The role of hadronization corrections

Bottom line: need better MC’s + hadronization models/calibration in $e^+e^-$

In a perfect world

- Parton showers with NNLL logarithmic accuracy matched to NNLO
- Hadronization models calibrated from scratch with many different observables, since current models were tuned using MC’s with lower accuracy

Alternatively

- Need a (much) more refined analytical understanding of non-perturbative corrections, for recent advances see e.g.,
- Look for better observables with smaller hadronization corrections, e.g., groomed event shapes
Conclusions

So where do we stand?

- No new data foreseen in the near future, so would including more perturbative orders (fixed order and/or resummation) improve precision without any new data? Not by itself. More perturbative orders alone are not likely to dramatically improve the precision of strong coupling extractions from existing data.

- If not, what are the limiting factors for precision in future QCD studies?

Main limiting factors are: systematics related to the estimation of hadronization corrections as well as the quality and consistency of current data.

- What should be done to eliminate those factors?

In addition to advancing the perturbative predictions, we must seriously refine our understanding/modeling of non-perturbative effects. This would be aided greatly by dedicated low-energy (below the Z-peak) measurements at future $e^+e^-$ facilities.
Thank you for your attention!
Backup slides
Hadronization corrections: simultaneous corrections for $R_2$ and $R_3$

**Challenge:** simultaneous corrections for $R_2$ and $R_3$

- hadronization corrections derived on a bin-by-bin basis, $R_{n,\text{hadron}} = R_{n,\text{parton}} f_n(y)$, $n = 2, 3, 4, \ldots$ can violate physical constraints: $0 \leq R_n \leq 1$ and $\sum_n R_n = 1$

**Solution:**

- introduce $\xi_1$ and $\xi_2$ such that at parton level $R_{2,\text{parton}} + R_{3,\text{parton}} + R_{\geq 4,\text{parton}} = 1$

\[
R_{2,\text{parton}} = \cos^2 \xi_1, \quad R_{3,\text{parton}} = \sin^2 \xi_1 \cos^2 \xi_2, \quad R_{\geq 4,\text{parton}} = \sin^2 \xi_1 \sin^2 \xi_2,
\]

- similarly at hadron level, set

\[
R_{2,\text{hadron}} = \cos^2(\xi_1 + \delta \xi_1), \quad R_{3,\text{hadron}} = \sin^2(\xi_1 + \delta \xi_1) \cos^2(\xi_2 + \delta \xi_2),
\]

\[
R_{\geq 4,\text{hadron}} = \sin^2(\xi_1 + \delta \xi_1) \sin^2(\xi_2 + \delta \xi_2)
\]

- the functions $\delta \xi_1(y)$ and $\delta \xi_2(y)$ account for hadronization corrections and are extracted from the MC samples

**This approach clearly preserves physical constraints**
Hadronization corrections: $\delta \xi_1(y)$ and $\delta \xi_2(y)$

- to avoid binning effects, the hadronization corrections are parametrized with smooth functions
- vertical lines show the fit ranges for the reference fits of $R_2$ and $R_3$
Hadronization corrections: hadron to parton ratios

- to avoid binning effects, the hadronization corrections are parametrized with smooth functions
- vertical lines show the fit ranges for the reference fits of $R_2$ and $R_3$
$R_2$ fits

Fit of $\alpha_s(M_Z)$ from experimental data for $R_2$ obtained using $N^3$LO and $N^3$LO+NNLL predictions for $R_2$. The reported uncertainty comes from MINUIT2.

<table>
<thead>
<tr>
<th>Fit ranges, log y Hadronization</th>
<th>$N^3$LO $\chi^2/\text{ndof}$</th>
<th>$N^3$LO+NNLL $\chi^2/\text{ndof}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[-1.75 + \mathcal{L}, -1]$ $S^C$</td>
<td>$0.12121 \pm 0.00095$</td>
<td>$0.11849 \pm 0.00092$</td>
</tr>
<tr>
<td></td>
<td>$20/86 = 0.24$</td>
<td>$20/86 = 0.24$</td>
</tr>
<tr>
<td>$[-2 + \mathcal{L}, -1]$ $S^C$</td>
<td>$0.12114 \pm 0.00081$</td>
<td>$0.11864 \pm 0.00075$</td>
</tr>
<tr>
<td></td>
<td>$26/100 = 0.26$</td>
<td>$26/100 = 0.26$</td>
</tr>
<tr>
<td>$[-2.25 + \mathcal{L}, -1]$ $S^C$</td>
<td>$0.12119 \pm 0.00060$</td>
<td>$0.11916 \pm 0.00063$</td>
</tr>
<tr>
<td></td>
<td>$44/150 = 0.29$</td>
<td>$44/150 = 0.29$</td>
</tr>
<tr>
<td>$[-2.5 + \mathcal{L}, -1]$ $S^C$</td>
<td>$0.12217 \pm 0.00052$</td>
<td>$0.12075 \pm 0.00055$</td>
</tr>
<tr>
<td></td>
<td>$89/180 = 0.50$</td>
<td>$107/180 = 0.59$</td>
</tr>
</tbody>
</table>

| $[-1.75 + \mathcal{L}, -1]$ $H^C$ | $0.11957 \pm 0.00098$ | $0.11698 \pm 0.00093$ |
|                                 | $22/86 = 0.26$ | $22/86 = 0.25$ |
| $[-2 + \mathcal{L}, -1]$ $H^C$  | $0.11923 \pm 0.00079$ | $0.11687 \pm 0.00076$ |
|                                 | $29/100 = 0.29$ | $28/100 = 0.28$ |
| $[-2.25 + \mathcal{L}, -1]$ $H^C$ | $0.11868 \pm 0.00068$ | $0.11679 \pm 0.00064$ |
|                                 | $43/150 = 0.28$ | $40/150 = 0.27$ |
| $[-2.5 + \mathcal{L}, -1]$ $H^C$ | $0.11849 \pm 0.00050$ | $0.11723 \pm 0.00053$ |
|                                 | $58/180 = 0.32$ | $58/180 = 0.32$ |

| $[-1.75 + \mathcal{L}, -1]$ $H^L$ | $0.12171 \pm 0.00109$ | $0.11897 \pm 0.00092$ |
|                                 | $21/86 = 0.25$ | $21/86 = 0.24$ |
| $[-2 + \mathcal{L}, -1]$ $H^L$  | $0.12144 \pm 0.00078$ | $0.11893 \pm 0.00075$ |
|                                 | $28/100 = 0.28$ | $26/100 = 0.26$ |
| $[-2.25 + \mathcal{L}, -1]$ $H^L$ | $0.12080 \pm 0.00069$ | $0.11881 \pm 0.00063$ |
|                                 | $43/150 = 0.28$ | $39/150 = 0.26$ |
| $[-2.5 + \mathcal{L}, -1]$ $H^L$ | $0.12024 \pm 0.00051$ | $0.11897 \pm 0.00053$ |
|                                 | $57/180 = 0.32$ | $52/180 = 0.29$ |
Simultaneous fit of $\alpha_s(M_Z)$ from experimental data for $R_2$ and $R_3$ obtained using N$^3$LO and N$^3$LO+NNLL predictions for $R_2$ and NNLO predictions for $R_3$. The reported uncertainty comes from MINUIT2.

<table>
<thead>
<tr>
<th>Fit ranges, log $y$ Hadronization</th>
<th>N$^3$LO $\chi^2$/ndof</th>
<th>N$^3$LO+NNLL $\chi^2$/ndof</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[-1.75 + \mathcal{L}, -1]$</td>
<td>$[1.5 + \mathcal{L}, -1]$</td>
<td>0.12195 ± 0.00072</td>
</tr>
<tr>
<td>$S^C$</td>
<td>120/143 = 0.84</td>
<td>140/143 = 0.98</td>
</tr>
<tr>
<td>$[-2 + \mathcal{L}, -1]$</td>
<td>$[1.75 + \mathcal{L}, -1]$</td>
<td>0.12163 ± 0.00061</td>
</tr>
<tr>
<td>$S^C$</td>
<td>153/187 = 0.82</td>
<td>176/187 = 0.94</td>
</tr>
<tr>
<td>$[-2.25 + \mathcal{L}, -1]$</td>
<td>$[2 + \mathcal{L}, -1]$</td>
<td>0.12075 ± 0.00044</td>
</tr>
<tr>
<td>$S^C$</td>
<td>208/251 = 0.83</td>
<td>222/251 = 0.88</td>
</tr>
<tr>
<td>$[-2.5 + \mathcal{L}, -1]$</td>
<td>$[2.25 + \mathcal{L}, -1]$</td>
<td>0.12143 ± 0.00043</td>
</tr>
<tr>
<td>$S^C$</td>
<td>321/331 = 0.97</td>
<td>336/331 = 1.01</td>
</tr>
<tr>
<td>$[-1.75 + \mathcal{L}, -1]$</td>
<td>$[1.5 + \mathcal{L}, -1]$</td>
<td>0.12068 ± 0.00073</td>
</tr>
<tr>
<td>$H^C$</td>
<td>126/143 = 0.88</td>
<td>147/143 = 1.03</td>
</tr>
<tr>
<td>$[-2 + \mathcal{L}, -1]$</td>
<td>$[1.75 + \mathcal{L}, -1]$</td>
<td>0.12006 ± 0.00061</td>
</tr>
<tr>
<td>$H^C$</td>
<td>163/187 = 0.87</td>
<td>188/187 = 1.01</td>
</tr>
<tr>
<td>$[-2.25 + \mathcal{L}, -1]$</td>
<td>$[2 + \mathcal{L}, -1]$</td>
<td>0.11869 ± 0.00043</td>
</tr>
<tr>
<td>$H^C$</td>
<td>221/251 = 0.88</td>
<td>238/251 = 0.95</td>
</tr>
<tr>
<td>$[-2.5 + \mathcal{L}, -1]$</td>
<td>$[2.25 + \mathcal{L}, -1]$</td>
<td>0.11845 ± 0.00045</td>
</tr>
<tr>
<td>$H^C$</td>
<td>302/331 = 0.91</td>
<td>310/331 = 0.94</td>
</tr>
<tr>
<td>$[-1.75 + \mathcal{L}, -1]$</td>
<td>$[1.5 + \mathcal{L}, -1]$</td>
<td>0.12248 ± 0.00068</td>
</tr>
<tr>
<td>$H^L$</td>
<td>121/143 = 0.85</td>
<td>141/143 = 0.99</td>
</tr>
<tr>
<td>$[-2 + \mathcal{L}, -1]$</td>
<td>$[1.75 + \mathcal{L}, -1]$</td>
<td>0.12211 ± 0.00057</td>
</tr>
<tr>
<td>$H^L$</td>
<td>155/187 = 0.83</td>
<td>180/187 = 0.96</td>
</tr>
<tr>
<td>$[-2.25 + \mathcal{L}, -1]$</td>
<td>$[2 + \mathcal{L}, -1]$</td>
<td>0.12071 ± 0.00044</td>
</tr>
<tr>
<td>$H^L$</td>
<td>209/251 = 0.83</td>
<td>227/251 = 0.90</td>
</tr>
<tr>
<td>$[-2.5 + \mathcal{L}, -1]$</td>
<td>$[2.25 + \mathcal{L}, -1]$</td>
<td>0.12041 ± 0.00044</td>
</tr>
<tr>
<td>$H^L$</td>
<td>266/331 = 0.80</td>
<td>278/331 = 0.84</td>
</tr>
</tbody>
</table>
Consistency tests

Several consistency tests performed

- simultaneous fit of $R_2 + R_3$ (see above)
- separate $R_3$ fit
- variation of $\chi^2$ definition
- change of fit ranges

- multiplicative hadronization corrections
- Sherpa MC hadronization $S^C$
- stability across $\sqrt{s}$ (see below)
- exclusion of data with $\sqrt{s} < M_Z$

 ![Graph showing $\alpha_s(M_Z)$ as a function of $\sqrt{s}$, GeV, with different curves for various hadronization corrections.](image-url)
Correlations: $\alpha_s(M_Z)$ vs. $\alpha_0(2\text{ GeV})$

Correlations between $\alpha_s(M_Z)$ and $\alpha_0(2\text{ GeV})$

- contours correspond to 1-, 2- and 3 standard deviations obtained in the fit
- systematic uncertainties not included