

DETERMINATION OF THE STRONG COUPLING
BEYOND NNLO USING EVENT SHAPE AVERAGES*

ADAM KARDOS

Department of Experimental Physics, Institute of Physics
Faculty of Science and Technology
University of Debrecen 4010 Debrecen, P.O. Box 105, Hungary

GÁBOR SOMOGYI

Wigner Research Centre for Physics
Konkoly-Thege Miklós u. 29-33, 1121 Budapest, Hungary

ANDRII VERBYTSKYI

Max-Planck-Institut für Physik, 80805 Munich, Germany

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We present a method of extracting the strong coupling at $N^3\text{LO}$ precision in QCD using a combination of $\mathcal{O}(\alpha_s^3)$ perturbative calculations with estimations of the $\mathcal{O}(\alpha_s^4)$ corrections from data. We apply the procedure to a set of event shape averages measured at the LEP, PETRA, PEP, and TRISTAN colliders. We account for non-perturbative effects using both modern Monte Carlo event generators as well as analytic models. Our results show that the precision of α_s extraction cannot be significantly improved solely with higher-order perturbative QCD predictions, but requires also a significant refinement of the understanding and modeling of the hadronization process.

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1. Introduction

The study of fully hadronic final states in electron–positron annihilation presents one of the cleanest approaches to measuring the strong coupling, $\alpha_s(M_Z)$. Such measurements have a rich history and in the past numerous

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extractions of the strong coupling have been performed by comparing experimental data on event shapes and jet rates to perturbative QCD predictions. Nowadays, progress in these measurements is driven solely by improvements in the theoretical description, given the current lack of active high-energy e^+e^- experiments. Nevertheless, some recent determinations have reached a relative precision of $\sim 1\%$ on $\alpha_S(M_Z)$ [1–3]. Having said that, examining the full set of e^+e^- determinations that enter the current world average [4], it is evident that there is a sizable spread between individual measurements.

In order to unravel the possible sources of these discrepancies, it is useful to catalogue the main differences between the determinations. To understand what is perhaps the most fundamental difference, recall that although experiments detect hadrons, perturbative QCD computations are performed with partons as basic degrees of freedom. Thus, in any comparison of experimental data to theoretical predictions, the parton-to-hadron transition must be modeled in one way or another, and theory calculations must be corrected for the effects of hadronization. There are fundamentally two different approaches to obtain these corrections: they may be computed using analytic models or extracted from simulations using Monte Carlo event generators. The first basic difference between various strong coupling measurements relates to the choice of hadronization modeling. Second, the amount of perturbative information included in the used theoretical predictions is also a source of difference. Currently, fully differential calculations are available for the $e^+e^- \rightarrow 3$ jets process at $\mathcal{O}(\alpha_S^3)$ accuracy, corresponding to the next-to-next-to-leading order (NNLO) of perturbation theory for three-jet observables [5–10]. Hence, current determinations use at least NNLO accurate theoretical predictions, however, for specific observables, notably the two-jet rate R_2 , this order in α_S actually corresponds to N³LO accuracy [3]. Moreover, further perturbative information is available in the form of resummed predictions. However, the accuracy of resummation that can be achieved varies from observable to observable, from as low as only next-to-leading logarithmic (NLL) in the three-jet rate R_3 [11] to NNLL in the logarithm of the two-jet rate R_2 [12], to N³LL for event shapes such as thrust [1] and the C -parameter [13]. Finally, the choice of observable itself can impact the results. For example, jet rates are known to be less sensitive to hadronization corrections than event shapes, but as we have just seen, the resummation for some event shapes can be carried to higher logarithmic orders than for jet rates. Clearly, there is no unique “best” observable.

This state of affairs then raises some interesting questions. First, given that new e^+e^- data are not foreseen in the near future, it is important to assess which improvements of the theoretical description are most relevant for further improvements of the measurements. In particular, would the availability of perturbative predictions at yet higher orders improve the precision

of α_S extraction without new data? If not, what are the limiting factors for precision in future QCD studies and what should be done to eliminate them? In order to address these questions, we perform a state-of-the-art perturbative QCD analysis with estimations of unknown higher-order perturbative corrections from data. We also employ both modern Monte Carlo tools as well as analytic models to determine hadronization corrections, the latter being extended to $\mathcal{O}(\alpha_S^4)$ accuracy for the first time. This allows us to study the impact of the choice of hadronization modeling in a broad sense.

In order to implement our analysis, it is obviously important to consider observables where the number of unknown higher-order perturbative coefficients that must be estimated from data is small. Hence, we turn to event shape averages and, in particular, consider the averages of one minus thrust and the C -parameter. Our choice of these particular event shapes is motivated by the abundance of available measurements. We note that while several measurements exist also for higher moments of event shapes, unfortunately almost all analyses fail to give information on the correlations between the various moments. However, these correlations are known to be strong [14] and thus a simultaneous fit of all of the available data would require taking them into account. Hence, we limit the analysis to only the first moments, *i.e.*, averages of event shapes.

2. Theoretical predictions

The n^{th} moment of an event shape variable O is defined by

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

where σ_{tot} denotes the total hadronic cross section in electron–positron annihilation, while $[O_{\min}, O_{\max}]$ is the kinematically allowed range of the observable O . On the other hand, the fixed-order perturbative predictions for $\langle O^n \rangle$ are usually presented normalized to the leading order hadronic cross section. At some reference renormalization scale $\mu = \mu_0$, we have

$$\begin{aligned} \frac{1}{\sigma_0} \int_{O_{\min}}^{O_{\max}} O^n \frac{d\sigma(O)}{dO} dO &= \frac{\alpha_S(\mu_0)}{2\pi} A_0^{\langle O^n \rangle} + \left(\frac{\alpha_S(\mu_0)}{2\pi} \right)^2 B_0^{\langle O^n \rangle} \\ &\quad + \left(\frac{\alpha_S(\mu_0)}{2\pi} \right)^3 C_0^{\langle O^n \rangle} + \left(\frac{\alpha_S(\mu_0)}{2\pi} \right)^4 D_0^{\langle O^n \rangle} + \mathcal{O}(\alpha_S^5). \end{aligned} \quad (2)$$

The first three coefficients in this equation (*i.e.*, $A_0^{\langle O^n \rangle}$, $B_0^{\langle O^n \rangle}$, and $C_0^{\langle O^n \rangle}$) have been known for some time [6, 8], however for this work, we have re-computed them with high numerical precision using the CoLoRFulNNLO method [10, 15, 16], see Table 1. Predictions for event shape averages normalized to the total hadronic cross section at any scale can be computed from Eq. (2) using the known expression for σ_{tot} and the renormalization group equation for the strong coupling, see Ref. [17] for details.

Table 1. The LO, NLO, and NNLO coefficients for the averages of one minus thrust and the C -parameter. For the details of the analytic calculation, see Ref. [17].

Coefficient	This work	Analytic	Ref. [6]	Ref. [8]
$A_0^{\langle(1-T)^1\rangle}$	2.1034(1)	2.10347	2.1035	2.10344(3)
$B_0^{\langle(1-T)^1\rangle}$	44.995(1)		44.999(2)	44.999(5)
$C_0^{\langle(1-T)^1\rangle}$	979.6(6)		867(21)	1100(30)
$A_0^{\langle C^1 \rangle}$	8.6332(5)	8.63789	8.6379	8.6378(1)
$B_0^{\langle C^1 \rangle}$	172.834(5)	172.859	172.778(7)	172.8(3)
$C_0^{\langle C^1 \rangle}$	3525(3)		3212(89)	4200(100)

We take into account b -quark mass corrections at NLO accuracy by subtracting the fraction of b -quark events from the massless coefficients and adding back the corresponding massive results obtained with the Zbb4 program [18]

$$\begin{aligned}
A^{\langle O^n \rangle} &= (1 - r_b(Q))A_{m_b=0}^{\langle O^n \rangle} + r_b(Q)A_{m_b \neq 0}^{\langle O^n \rangle}, \\
B^{\langle O^n \rangle} &= (1 - r_b(Q))B_{m_b=0}^{\langle O^n \rangle} + r_b(Q)B_{m_b \neq 0}^{\langle O^n \rangle}.
\end{aligned} \tag{3}$$

Above $r_b(Q)$ is the fraction of b -quark events which is given by

$$r_b(Q) = \frac{\sigma_{m_b \neq 0}(e^+e^- \rightarrow b\bar{b})}{\sigma_{m_b \neq 0}(e^+e^- \rightarrow \text{hadrons})}. \tag{4}$$

Finally, as discussed in Introduction, the $\mathcal{O}(\alpha_S^4)$ corrections, *i.e.*, the $D_0^{\langle O^n \rangle}$ coefficients, are extracted from data together with $\alpha_S(M_Z)$. With regard to this extraction, we emphasize that its main point is not to obtain an accurate determination of these quantities. Rather, it is to model them as best as possible in the absence of an actual computation, so that we can assess the impact of including terms beyond NNLO accuracy in determinations of the strong coupling.

3. Hadronization corrections

The modeling of non-perturbative corrections is essential in order to perform a meaningful comparison of theoretical predictions with data. In this analysis, we pursue two approaches to describing hadronization.

First, hadronization corrections can be extracted from Monte Carlo event generators. Thus, we generate samples of $e^+e^- \rightarrow Z/\gamma \rightarrow 2, 3, 4, 5$ parton processes using **MadGraph5** [19] and the **OpenLoops** [20] one-loop library. The two-parton final process is computed at NLO accuracy. The events are then showered and hadronized using different parton showers and hadronization models. In our default setup, labeled H^L , we use **Herwig7.2.0** [21] and employ the Lund fragmentation model [22] to describe the parton-to-hadron transition. To study the systematics associated with the choice of hadronization model, we also generate predictions with **Herwig7.2.0** and the cluster hadronization model [23] (H^C setup). Finally, for cross-checks, we consider results obtained using **Sherpa2.2.8** [24] with the cluster hadronization model [25] (S^C setup). Then in each setup, we compute predictions for event shape averages both at hadron ($\langle O^n \rangle_{\text{MC hadrons}}$) and parton levels ($\langle O^n \rangle_{\text{MC partons}}$). In order to account for the presence of a shower cut-off scale of $Q_0 \simeq \mathcal{O}(1 \text{ GeV})$ in the Monte Carlo programs which effects event shape distributions (see *e.g.*, Refs. [26, 27]), we compute each prediction for several different values of this cut-off and extrapolate the results to $Q_0 \rightarrow 0 \text{ GeV}$. Theory predictions are then corrected for hadronization by the ratio of hadron-to-parton level Monte Carlo results

$$\langle O^n \rangle_{\text{corrected}} = \langle O^n \rangle_{\text{theory}} \times \frac{\langle O^n \rangle_{\text{MC hadrons}, Q_0=0 \text{ GeV}}}{\langle O^n \rangle_{\text{MC partons}, Q_0=0 \text{ GeV}}}. \quad (5)$$

Figure 1 shows the Monte Carlo predictions at both hadron and parton level extrapolated to $Q_0 \rightarrow 0 \text{ GeV}$ as well as the perturbative result at NNLO together with the measured data. The hadron and parton level Monte Carlo predictions provide reasonable descriptions of the data and NNLO results for a wide range of center-of-mass energies. However, the parton level Monte Carlo results are not reliable for the lowest values of \sqrt{s} , since in QCD the event shape moments $\langle O^n \rangle$ should decrease with energy. Thus, measurements with $\sqrt{s} < 29 \text{ GeV}$ are excluded from the analysis.

Second, non-perturbative corrections can also be computed using analytic models. In the dispersive model of hadronization corrections considered here, the perturbative event shape averages are simply shifted

$$\langle O^1 \rangle_{\text{hadrons}} = \langle O^1 \rangle_{\text{hadrons}} + a_O \mathcal{P}. \quad (6)$$

Here, a_O is an observable-specific constant with $a_{1-T} = 2$ and $a_C = 3\pi$,

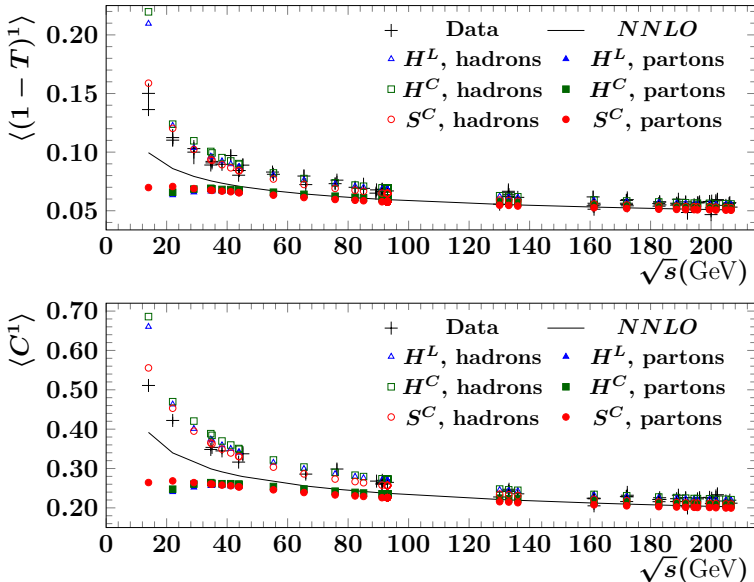


Fig. 1. Data and predictions of the Monte Carlo event generators extrapolated to $Q_0 \rightarrow 0$ GeV. The NNLO result was computed using $\alpha_S(M_Z) = 0.118$.

while \mathcal{P} is the power correction which is universal for all event shapes¹. In our analysis, we must compute \mathcal{P} to $\mathcal{O}(\alpha_S^4)$ accuracy. The ingredients of this computation are the known four-loop running of the strong coupling in the $\overline{\text{MS}}$ scheme and the relation between the effective soft coupling in the Catani–Marchesini–Webber (CMW) scheme α_S^{CMW} and the strong coupling in the $\overline{\text{MS}}$ scheme α_S . This relation has the general form of

$$\alpha_S^{\text{CMW}} = \alpha_S \left[1 + \frac{\alpha_S}{2\pi} K + \left(\frac{\alpha_S}{2\pi} \right)^2 L + \left(\frac{\alpha_S}{2\pi} \right)^2 M + \mathcal{O}(\alpha_S^4) \right], \quad (7)$$

where K is simply the one-loop cusp anomalous dimension, while L and M can be computed once the effective soft coupling is explicitly defined beyond NLL accuracy. As there are several proposals in the literature for this definition [28, 29], the L and M coefficients carry an associated scheme dependence. We denote by A^0 and A^T the schemes based on the definitions $\mathcal{A}_{0,i}$ and $\mathcal{A}_{T,i}$ of Ref. [29]². We also define the A^{cusp} scheme for easier comparison to previous work [30]. This scheme corresponds to simply setting L and M equal to the two- and three-loop cusp anomalous dimensions. The power correction \mathcal{P} at N³LO accuracy takes the form of

¹ See Ref. [17] for some comments on possible limitations of this model.

² The definition of the soft coupling in Ref. [28] is equivalent to $\mathcal{A}_{T,i}$ of Ref. [29].

$$\begin{aligned}
 \mathcal{P}(\alpha_S, Q, \alpha_0) = & \frac{4C_F}{\pi^2} \mathcal{M} \frac{\mu_I}{Q} \left\{ \alpha_0(\mu_I) - \left[\alpha_S(\mu_R) + \left(K + \beta_0 \left(1 + \ln \frac{\mu_R}{\mu_I} \right) \right) \right] \right. \\
 & \times \frac{\alpha_S^2(\mu_R)}{2\pi} + \left(2L + (4\beta_0(\beta_0 + K) + \beta_1) \left(1 + \ln \frac{\mu_R}{\mu_I} \right) + 2\beta_0^2 \ln^2 \frac{\mu_R}{\mu_I} \right) \frac{\alpha_S^3(\mu_R)}{8\pi^2} \\
 & + \left(4M + (2\beta_0(12\beta_0(\beta_0 + K) + 5\beta_1) + \beta_2 + 4\beta_1 K + 12\beta_0 L) \left(1 + \ln \frac{\mu_R}{\mu_I} \right) \right. \\
 & \left. \left. + \beta_0(12\beta_0(\beta_0 + K) + 5\beta_1) \ln^2 \frac{\mu_R}{\mu_I} + 4\beta_0^3 \ln^3 \frac{\mu_R}{\mu_I} \right) \frac{\alpha_S^4(\mu_R)}{32\pi^3} \right] \left. \right\}, \quad (8)
 \end{aligned}$$

where \mathcal{M} is the so-called Milan factor and μ_I is the scale at which the perturbative and non-perturbative couplings are matched³. Following the traditional choice, we set $\mu_I = 2$ GeV. Finally, $\alpha_0(\mu_I)$ denotes the first moment of the effective soft coupling below the scale μ_I

$$\alpha_0(\mu_I) = \frac{1}{\mu_I} \int_0^{\mu_I} d\mu \alpha_S^{\text{CMW}}(\mu) \quad (9)$$

and is a non-perturbative (and scheme-dependent) parameter of the model.

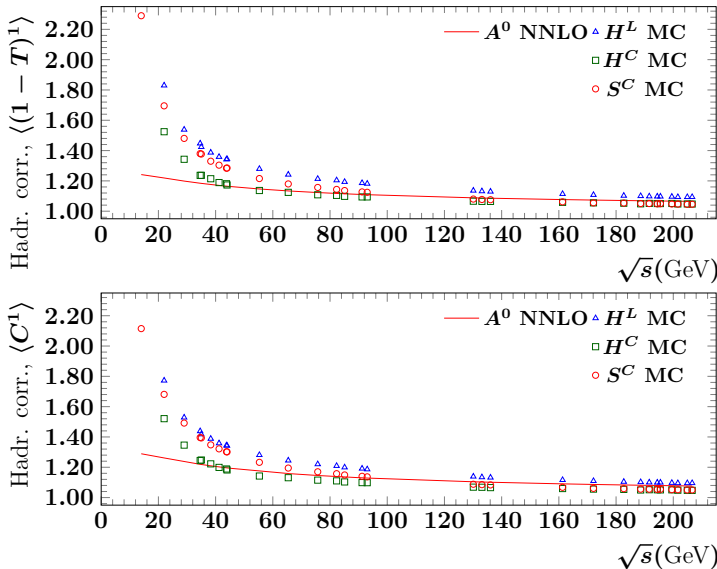


Fig. 2. Multiplicative hadronization corrections extracted from Monte Carlo event generators and the analytic hadronization model in the A^0 scheme. The hadronization corrections in the A^T and A^{cusp} schemes are numerically very similar to the A^0 scheme and are not shown.

³ The subscripts on the scales μ_R and μ_I stand for “renormalization” and “infrared”, respectively.

Figure 2 shows the ratios of hadron-to-parton level predictions for the various hadronization models we consider. Note that hadronization corrections from the A^T and A^{cusp} scheme are numerically very close to those of the A^0 scheme and are thus not shown separately.

4. Data sets and fit procedure

For the analysis, we considered measurements from the ALEPH, AMY, DELPHI, HRS, JADE, L3, MARK, MARKII, OPAL, and TASSO experiments. Our combined analysis includes over 20 data sets spanning a wide range of center-of-mass energies between 29 GeV and 206 GeV, see Ref. [17] for details. Our selection of the variables $\langle(1-T)^1\rangle$ and $\langle C^1\rangle$ (*i.e.*, averages of one minus thrust and the C -parameter) was explained at the end of Introduction.

In order to determine the optimal values of $\alpha_S(M_Z)$, we used the MINUIT2 program to minimize the function

$$\chi^2(\alpha_S) = \sum_i^{\text{all data sets}} \chi_i^2(\alpha_S), \quad (10)$$

where for each data set i , we have $\chi_i^2(\alpha_S) = (\vec{D} - \vec{P}(\alpha_S))V^{-1}(\vec{D} - \vec{P}(\alpha_S))^T$. Here, \vec{D} and $\vec{P}(\alpha_S)$ denote the vectors of data points and calculated pre-

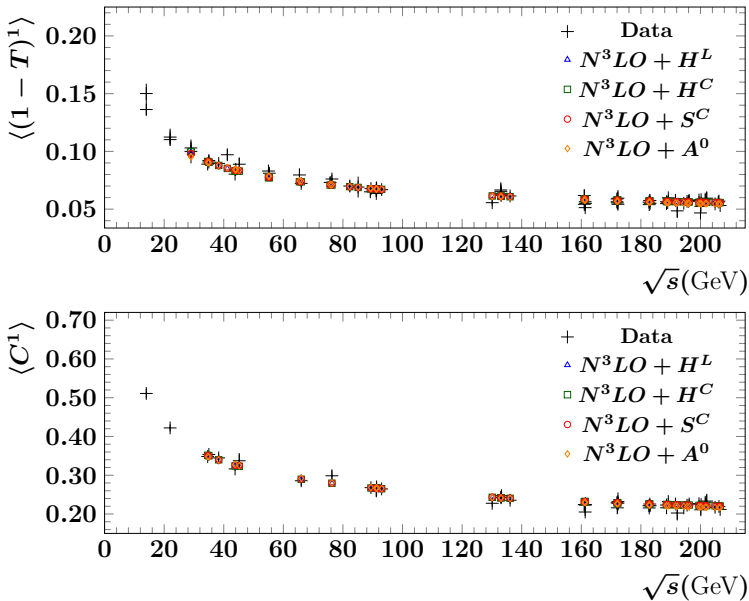


Fig. 3. Data and fits to the data using perturbative predictions at N^3LO accuracy and different hadronization models.

dictions, while V stands for the covariance matrix of \vec{D} . In this analysis, V was diagonal with the values of the diagonal elements obtained by adding statistical and systematic uncertainties in quadrature for each measurement.

In addition to $\alpha_S(M_Z)$, we fit also the $\mathcal{O}(\alpha_S^4)$ perturbative coefficients $D^{(O^n)}$ in $N^3\text{LO}$ fits, as well as the value of $\alpha_0(2\text{ GeV})$ when using the analytic hadronization model. Moreover, the Milan factor is also included in the fit as a constrained parameter, which provides a way to take into account its theoretical uncertainty. The multiple numerical results of the NNLO and $N^3\text{LO}$ fits are presented in Ref. [17], while Fig. 3 shows the predictions for the $N^3\text{LO}$ fits for individual data points. Note that the dependence on the analytic hadronization scheme is mild and hence only the results for the A^0 scheme are shown.

5. Results

The values obtained for $\alpha_S(M_Z)$ in the various fits are presented in Fig. 4. Examining the figure, we observe good agreement between fits to $\langle(1-T)^1\rangle$ and $\langle C^1\rangle$ data both at NNLO and $N^3\text{LO}$ accuracy. This can be viewed as a check of the internal consistency of the extraction procedure. We also observe that the dependence of the fitted value of $\alpha_S(M_Z)$ on the analytic hadronization scheme is mild. However, similarly to previous studies [30], the discrepancy between the results obtained using Monte Carlo hadronization models and analytic hadronization models is found to be sizable both in the NNLO and the $N^3\text{LO}$ fits. This suggests that the discrepancy has a fundamental origin and would continue to hold even using exact $N^3\text{LO}$ predictions. Consequently a better understanding of hadronization is of basic importance to increasing the precision of $\alpha_S(M_Z)$ extractions in future studies.

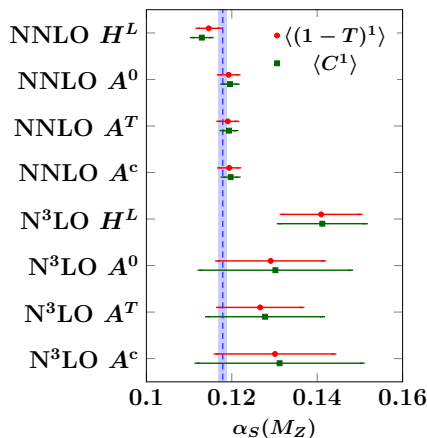


Fig. 4. Fitted values of $\alpha_S(M_Z)$ at NNLO and $N^3\text{LO}$ using different hadronization models.

Turning to the fits of the $\mathcal{O}(\alpha_S^4)$ perturbative coefficients $D^{\langle(1-T)^1\rangle}$ and $D^{\langle C^1\rangle}$, Fig. 5 shows that their extracted values are in reasonable agreement between fits using Monte Carlo and analytic hadronization models for both observables. This demonstrates the viability of extracting higher-order coefficients, once a large amount of precise and consistent data is available. Accurate high-energy measurements would be especially valuable for such an extraction.

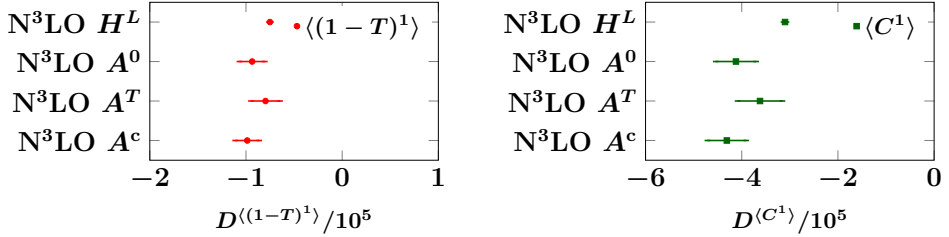


Fig. 5. Fitted values of the $\mathcal{O}(\alpha_S^4)$ perturbative coefficients $D^{\langle(1-T)^1\rangle}$ (left) and $D^{\langle C^1\rangle}$ (right) using different hadronization models.

Last, we examine the results of the fits for the non-perturbative parameter $\alpha_0(2\text{ GeV})$, presented in Fig. 6. Recall that this parameter is scheme-dependent, so the fitted values in the different schemes should not be directly compared to each other. Nevertheless, we see that the choice of scheme has only a small numerical impact on the extracted value of $\alpha_0(2\text{ GeV})$. Moreover, the results obtained from fits to $\langle(1-T)^1\rangle$ and $\langle C^1\rangle$ data agree well with each other both at NNLO and N³LO accuracy. The rather large uncertainties observed in the N³LO fits are due primarily to the insufficient amount of data, the quality of the available data and the extraction method itself.

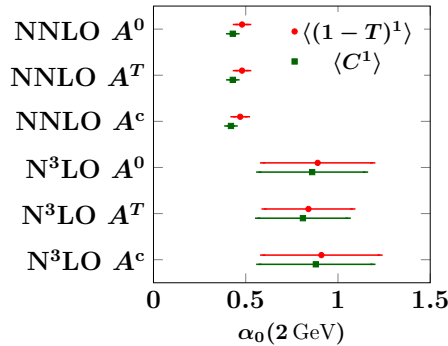


Fig. 6. Fitted values of the non-perturbative parameter $\alpha_0(2\text{ GeV})$ at NNLO and N³LO using different hadronization models.

6. Conclusions

The aim of the present analysis was to assess the factors that will determine the precision of QCD analyses of e^+e^- data once theoretical predictions at $\mathcal{O}(\alpha_S^4)$ accuracy become available. To this end, we have performed an extraction of $\alpha_S(M_Z)$ from the averages of the event shapes $\langle(1-T)^1\rangle$ and $\langle C^1\rangle$ at different perturbative orders and employed different types of hadronization models. Using perturbative predictions at NNLO accuracy and analytic hadronization models, we have obtained values of the strong coupling that are consistent with the latest world average $\alpha_S(M_Z)_{\text{PDG2020}} = 0.1179 \pm 0.0010$.

In order to determine the impact of the presently unknown $\mathcal{O}(\alpha_S^4)$ corrections on the measurement of the strong coupling, we estimated the missing perturbative coefficients from data. The values of $\alpha_S(M_Z)$ obtained in this way are compatible with the current world average, within somewhat large uncertainties, *e.g.*,

$$\alpha_S(M_Z)^{\text{N}^3\text{LO}+A^0} = 0.12911 \pm 0.00177 (\text{exp.}) \pm 0.0123 (\text{scale}) \quad (11)$$

from the $\langle(1-T)^1\rangle$ data. The obtained precision can be increased with more high-quality data from future experiments.

Finally, the comparison of results obtained with Monte Carlo and analytic hadronization models exhibits what appears to be a fundamental discrepancy which would likely continue to hold even if the exact $\mathcal{O}(\alpha_S^4)$ corrections were known. This suggests that future extractions of the strong coupling will be strongly affected by the modeling of hadronization corrections even once exact higher-order corrections are included in the analyses. Thus, in addition to advancing the perturbative predictions, our understanding and modeling of non-perturbative effects will need to be seriously refined in order to achieve substantial improvements in future extractions of the strong coupling. This would be aided greatly by dedicated low-energy (below the Z-peak) measurements at future e^+e^- facilities.

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