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The variable flavor number scheme to three-loop order*

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We describe the variable flavor number scheme to three-loop order, which modifies the massless parton densities by single- and two-mass effects and introduces heavy-quark parton distribution functions for charm and bottom. A renormalization group analysis shows the validity of this picture at large scales Q^2, where it resembles the non-power-suppressed heavy-flavor corrections completely. We also provide numerical implementations of a series of charged and neutral current Wilson coefficients.

Loops and Legs in Quantum Field Theory (LL2026)
12-17, April, 2026
Bayreuth, Germany

*DESY 26–064, RISC Report number 26-06, CERN-TH-2026-113, MPP-2026-89, PoS (LL2026) 025
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1. Introduction

The variable flavor number schemes (VFNS) account for the universal heavy-flavor contributions of the deep-inelastic (DIS) structure functions in the form of modified parton distribution functions. They are important for the matching at flavor thresholds. In the region of large virtualities $Q^2 \gg m_Q^2$, where m_Q denotes the heavy-quark mass, full account is given of all heavy-quark corrections, neglecting power corrections of $O((m_Q^2/Q^2)^k)$, $k \geq 1$. This is implemented by the renormalization group equation [1, 2]. Since the ratio of the charm and bottom quark masses is not small, one may consider the decoupling of two quarks at the same time. The single-mass VFNS has been introduced in Ref. [3] to two-loop order and two-loop two-mass effects were described in Refs. [4, 5]. The single-mass VFNS at three-loop order has been presented in Ref. [6, 7] in the unpolarized and polarized cases. The structure of the two-mass VFNS to three-loop orders was described in Ref. [8]. Using the VFNS, massless Wilson coefficients are paired with massive operator matrix elements (OMEs). This does not allow the description of power corrections arising in observables, which will become important in the kinematic region of virtualities Q^2 below a certain scale Q_0^2. For the structure function $F_2(x, Q^2)$ one has $Q_0^2 = 10\, m_Q^2$, cf. [9].

Some modifications of the single-mass VFNS have been discussed in the literature in Refs. [10–14], to second order. Also these approaches have to be shown to obey the renormalization group equation to construct observables using the respective modified parton distribution functions.

This paper is organized as follows. Basic relations of the VFNS are discussed in Section 2. In Section 3 the heavy-quark corrections to structure functions at large virtualities are described. Quantitative results on the single-mass heavy-quark effects on parton distribution functions are described in Section 4. The two-mass operator matrix elements are illustrated in Section 5 and Section 6 contains the conclusions.

2. Operator matrix elements and the VFNS

The massive OMEs, cf. Ref. [15], have all been calculated in the single- and two-mass cases to three-loop order. The one-loop corrections were obtained in Refs. [16, 17], the two-loop corrections in Refs. [3, 5, 9, 18–21]. At three-loop order the single-mass OMEs were calculated in Refs. [22–32] and in the two-mass case in Refs. [8, 33–37]. At one-loop order only the OMEs $A_{Qg}, A_{gg,Q}$ contribute, at two-loop order one further has $A_{qq,Q}^{\rm NS}, A_{Qq}^{\rm PS}, A_{gq,Q}$. Finally, at three-loop order there are also contributions due to $A_{qq,Q}^{\rm PS}, A_{qg,Q}$ in the single-mass case. If the first index contains only lower case letters, the local operators are placed on massless lines. The first two-mass contributions emerge at the two-loop level with factorizing contributions $A_{Qg}^{(1)} \cdot A_{gg,Q}^{(1)}$ [4, 5]. Genuine non-factorizing contributions first emerge at three-loop order $A_{qq,Q}^{\rm NS,two}, A_{Qq}^{\rm PS,two}, A_{Qg}^{\rm two}, A_{gq,Q}^{\rm two}, A_{gg,Q}^{\rm two}$, supplemented by factorizing contributions.

In the polarized case, we work in the Larin scheme [38], which requires to refer to parton distributions evolved in this scheme, cf. Ref. [39], and Wilson coefficients [40] or hard-scattering sub-system cross sections in this scheme to form observables.

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In Mellin space the parton densities in the two-flavor VFNS are obtained from the massless parton distributions by the following relations,

$$f_k(N_F+2) + f_{\overline{k}}(N_F+2) = A_{qq,Q}^{\mathrm{NS},+}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) \cdot \left[f_k(N_F) + f_{\overline{k}}(N_F)\right] + \frac{1}{N_F} A_{qq,Q}^{\mathrm{PS}}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) \cdot \Sigma^+(N_F) + \frac{1}{N_F} A_{qg,Q}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) \cdot G(N_F) \tag{1}$$

$$f_k(N_F+2) - f_{\overline{k}}(N_F+2) = A_{qq,Q}^{\mathrm{NS},-}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) \cdot \left[f_k(N_F) - f_{\overline{k}}(N_F)\right] \tag{2}$$

$$f_Q(N_F+2) + f_{\overline{Q}}(N_F+2) = A_{Qq}^{\mathrm{PS}}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \right) \cdot \Sigma^+(N_F) + A_{Qg}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) \cdot G(N_F) \tag{3}$$

$$f_c(N_F+1) - f_{\overline{c}}(N_F+1) = A_{Qq}^{\mathrm{PS,s}}\left(N_F, \frac{m_c^2}{\mu^2}\right) \cdot \Sigma^-(N_F) \tag{4}$$

$$f_b(N_F+1) - f_{\overline{b}}(N_F+1) = A_{Qq}^{\mathrm{PS,s}}\left(N_F, \frac{m_b^2}{\mu^2}\right) \cdot \Sigma^-(N_F) \tag{5}$$

$$\Sigma^+(N_F+2) = \left[A_{qq,Q}^{\mathrm{NS}}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) + A_{qq,Q}^{\mathrm{PS}}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) + A_{Qq}^{\mathrm{PS}}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right)\right] \times \Sigma^+(N_F) + \left[A_{qg,Q}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) + A_{Qg}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right)\right] \cdot G(N_F) \tag{6}$$

$$G(N_F+2) = A_{gq,Q}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) \cdot \Sigma^+(N_F) + A_{gg,Q}\left(N_F+2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) \cdot G(N_F)\,. \tag{7}$$

Here N_F denotes the number of light flavors, f_k are the light-quark densities and G denotes the gluon distribution. $A_{qq}^{\mathrm{NS},+}$ refers to the even and $A_{qq}^{\mathrm{NS},-}$ to the odd moments of A_{qq}^{NS} in the unpolarized case. The singlet distributions $\Sigma^\pm$ are given by

$$\Sigma^\pm = [u \pm \bar{u}] + [d \pm \bar{d}] + [s \pm \bar{s}]. \tag{8}$$

3. Heavy-quark corrections to structure functions at large virtualities

In the fixed flavor number scheme the asymptotic heavy-quark corrections to the structure function $F_2(x, Q^2)$, disregarding power corrections, are given by Eq. (10) of Ref. [41]. In the single-mass VFNS one obtains

$$F_2^{\mathrm{VFNS}}(x, Q^2) = \sum_{k=1}^{N_F} F_2^{\mathrm{VFNS},e_k^2}(x, Q^2) + \sum_{Q=c,b} F_2^{\mathrm{VFNS},e_Q^2}(x, Q^2), \tag{9}$$

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where

$$F_2^{\mathrm{VFNS},e_k^2}(x,Q^2) = e_k^2\Bigg[f_{k+\bar{k}}(x,Q^2,N_F+1)\otimes C_2^{\mathrm{NS}}\left(x,\frac{Q^2}{\mu^2},N_F+1\right)+\Sigma(x,\mu^2,N_F+1)$$
$$\otimes\tilde{C}_{2,q}^{\mathrm{PS}}\left(x,\frac{Q^2}{\mu^2},N_F+1\right)+G(x,\mu^2,N_F+1)\otimes\tilde{C}_{2,g}^{\mathrm{S}}\left(x,\frac{Q^2}{\mu^2},N_F+1\right)\Bigg], \tag{10}$$

$$F_2^{\mathrm{VFNS},e_Q^2}(x,Q^2) = e_Q^2\Bigg[f_{Q+\bar{Q}}(x,Q^2,N_F+1)\otimes C_2^{\mathrm{NS}}\left(x,\frac{Q^2}{\mu^2},N_F+1\right)+\Sigma(x,\mu^2,N_F+1)$$
$$\otimes\tilde{C}_{2,q}^{\mathrm{PS}}\left(x,\frac{Q^2}{\mu^2},N_F+1\right)+G(x,\mu^2,N_F+1)\otimes\tilde{C}_{2,g}^{\mathrm{S}}\left(x,\frac{Q^2}{\mu^2},N_F+1\right)\Bigg]. \tag{11}$$

Here the functions $C_{2,i}^{(k)}$ denote the massless Wilson coefficient [40, 42], with $\tilde{f}(N_F) = f(N_F)/N_F$. Applying the renormalization group operator to $F_2(x,Q^2)$

$$\left[\mu\frac{\partial}{\partial\mu}+\beta(g,N_F)\frac{\partial}{\partial g}\right]F_2(x,Q^2) = \frac{d}{dt}F(x,Q^2) = 0, \quad \text{with} \quad t = -2\ln\left(\frac{\mu_0^2}{\mu^2}\right) \tag{12}$$

results in

$$\delta F_2(x,Q^2) = F_2^{\mathrm{total}}(x,Q^2) - F_2^{\mathrm{VFNS}}(x,Q^2) = O(a_s^4), \tag{13}$$

where $a_s = \alpha_s/(4\pi)$ denotes the strong coupling constant. Thus the representation in the VFNS agrees to the one in the fixed flavor number scheme in the range of large values of Q^2 at three-loop accuracy.

4. Single-mass heavy-quark effects on parton distribution functions

We have designed numerical x-space codes for all unpolarized and polarized single-mass OMEs to three-loop order in `C++` and `Fortran` in Ref. [6]. In addition, we have released x-space codes for the massless and asymptotic massive Wilson coefficients to three-loop order in Refs. [41, 43]. The codes are very fast and precise and consist of analytic small- and large-x expansions and cubic splines over fine-grided data arrays for the remainder part, leaving a_s, $\ln(Q^2/\mu^2)$, $\ln(m_Q^2/\mu^2)$, N_F, and charge weights as free parameters. They can be efficiently used in QCD-fitting codes.

In Figure 1 we illustrate the pure single-mass heavy-flavor contributions divided by the massless contributions. We also show the degree of convergence from the $O(a_s)$ to $O(a_s^3)$ in the unpolarized case for the non-singlet, singlet and gluon distributions, as well as for the heavy-quark distribution functions.

Starting from three-loop order, there are also $f_Q - f_{\bar{Q}}$ distribution functions. These distributions turn out to be rather small, cf. Ref. [7], and are shown in Figure 2.[1]

[1] In the polarized case the associated three-loop anomalous dimension has been newly calculated by three different methods for the first time in Ref. [7] and independently in Ref. [44].

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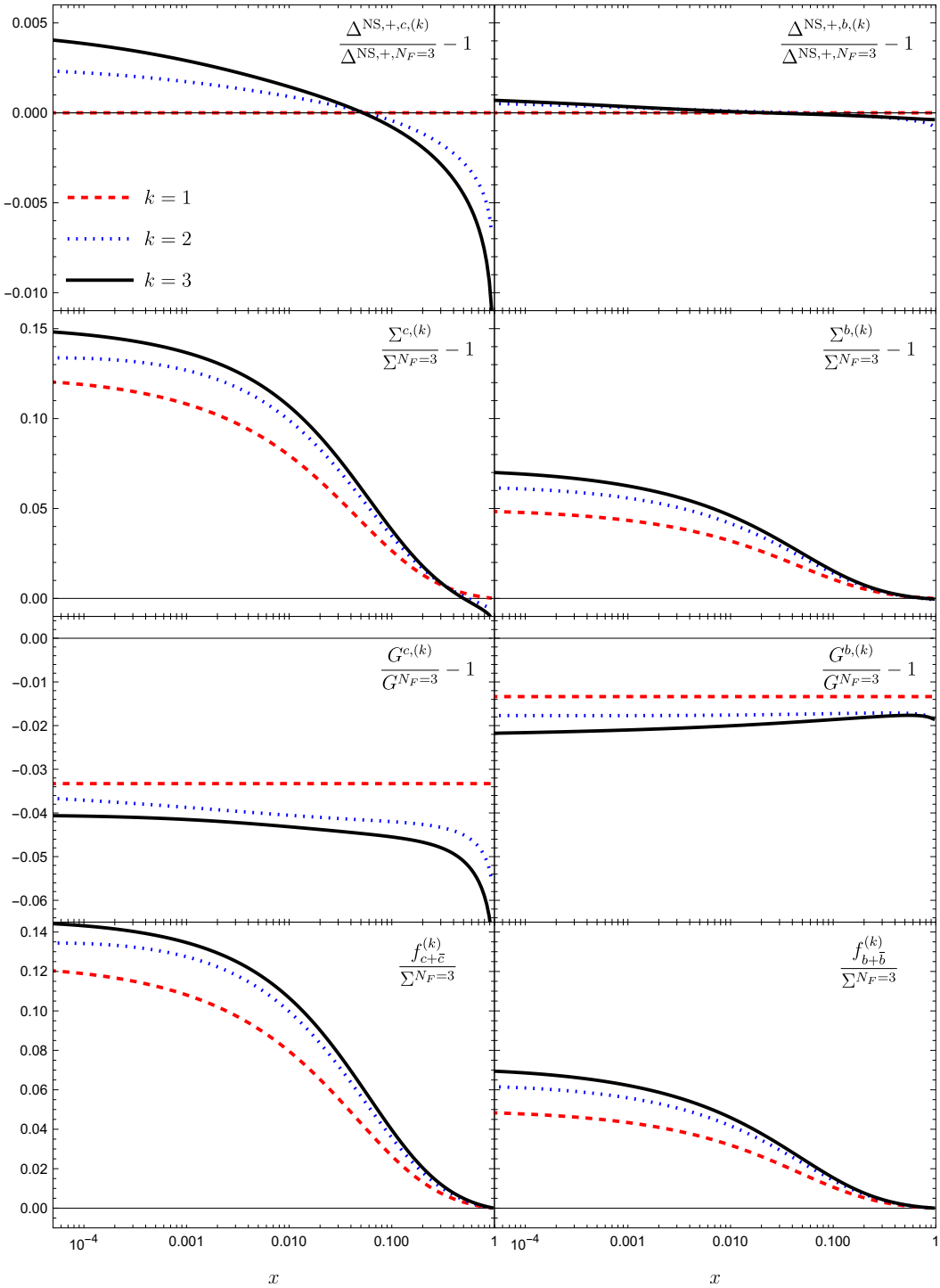


Figure 1: Left panels: relative heavy-quark contributions due to charm to $\Delta^{\rm NS,+}, \Sigma, G$ and $f_{c+\bar{c}}$. Right panels: relative heavy-quark contributions due to bottom to $\Delta^{\rm NS,+}, \Sigma, G$ and $f_{b+\bar{b}}$, both at $Q^2 = 100$ GeV^2. The massive OMEs have been truncated to the perturbative order $O(a_s^k)$. The denominators of the ratios are $\Sigma^{\rm N_F=3}$ or $G^{\rm N_F=3}$, respectively. Dashed lines: $O(a_s)$. Dotted lines: contributions to $O(a_s^2)$. Full lines: contributions to $O(a_s^3)$; from Ref. [6].

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Numerical results for the single-mass heavy-flavor three-loop Wilson coefficients of the structure functions $F_L(x,Q^2)$ [15, 19], $xF_3(x,Q^2)$ [45] and $g_1^{\rm NS}(x,Q^2)$ [46], as well as for the charged current structure functions $F_L^{W^+-W^-}(x,Q^2)$ and $F_2^{W^+-W^-}(x,Q^2)$ [47] and the unpolarized two-loop charged current structure functions [48] have been presented before.[2] We attach the corresponding codes as ancillary files to this paper. Here the same representation for the external variables as in Ref. [41] is used. The functions are provided in terms of harmonic polylogarithms [50, 51].[3]

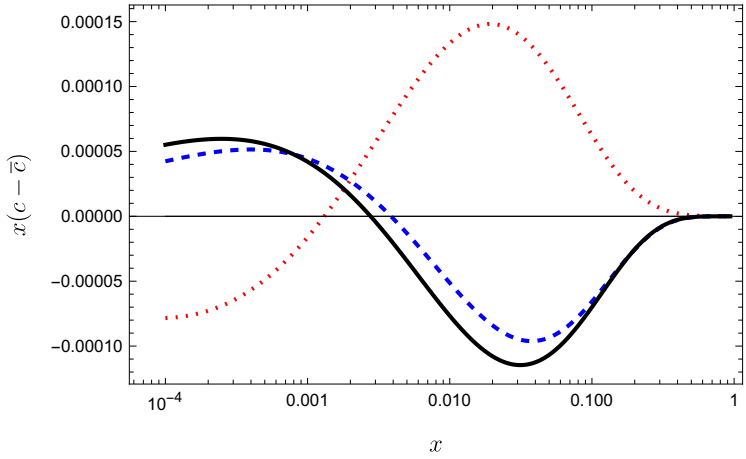


Figure 2: The unpolarized distributions $x[c(x,Q^2)-\overline{c}(x,Q^2)]$; from Ref. [7].

5. Two-mass operator matrix elements

The two-mass operator matrix elements were all calculated to three-loop order in the unpolarized and polarized cases. They consist of factorizable and, from three-loop order, also non-factorizable contributions. The emergence of two masses complicates the respective integrals and functional representation of the final results.[4] The respective contributions at three-loop order have color factors of $T_F^2 C_{F,A}$.[5] The relative impact of the two-mass corrections can be illustrated comparing to the complete contributions of $O(T_F^2 C_{F,A})$ in the respective case. We show this in Figure 3. The ratios are of the size $O(1/2)$. Precise numerical codes for the two-mass corrections will be released in the same form as in the single-mass case very soon.

6. Conclusions

The single- and two-mass VFNS has been promoted from two- to three-loop order both in the unpolarized and polarized case. The mass-modified parton distribution functions are uniquely

[2] We have corrected typographical errors in $H_{3,g}^{W,(2)}(x)$, [48], Eq. (C.11), and agree with Ref. [49]. Our N-space results were confirmed by Ref. [49].

[3] In the design of the `Fortran` programmes we used code optimization [52].

[4] For the calculation methods we refer to the original papers and the survey [53].

[5] In QCD the color factors are $T_F = 1/2, C_F = (N_c^2-1)/(2N_c), C_A = N_c, N_c = 3$.

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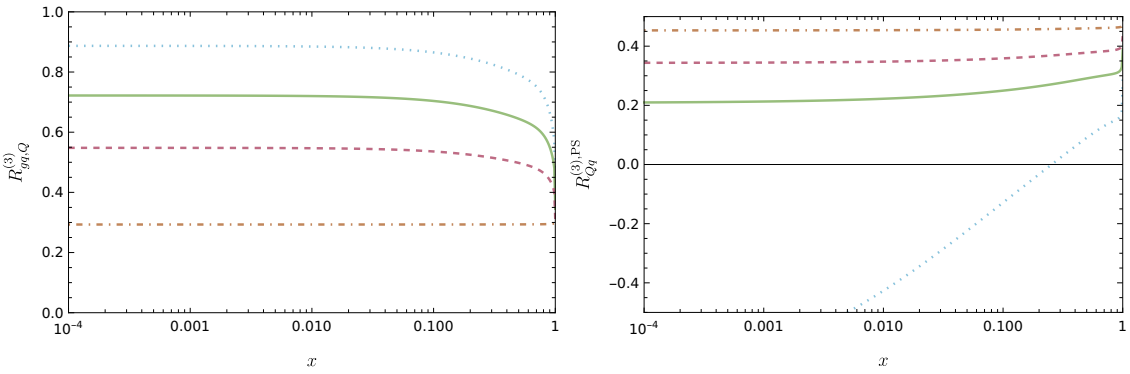


Figure 3: The contributions of the two-mass OMEs A_{gq}^{two} and $A_{Qq}^{\mathrm{two,PS}}$ normalized to the complete contributions $O(T_F^2)$ in the unpolarized case. Dotted lines: $Q^2 = 30\mathrm{GeV}^2$ Full lines: $Q^2 = 50\mathrm{GeV}^2$ Dashed lines: $Q^2 = 100\mathrm{GeV}^2$ Dash-dotted lines: $Q^2 = 1000\mathrm{GeV}^2$; from Refs. [33, 43].

implied by the massive renormalization group equation. These schemes describe the deep-inelastic structure functions in the region $Q^2 \gg m_Q^2$, where power corrections can be safely neglected.[6] Fast and precise numerical implementations were released as public codes for the use in data analyses in the massless and single-mass case [6]. This also applies to the massive three-loop Wilson coefficients [41] and the massless three-loop Wilson coefficients [43].

The present framework allows for more precise calculations of different processes for which the VFNS can be used. This applies in particular to processes at hadron colliders. A consistent treatment of the heavy-flavor corrections is of central importance for the measurement of the strong coupling constant a_s and the heavy-quark masses using high-energy processes at different colliders [56, 57], if gluon and flavor-singlet contributions are involved.

However, for a high-precision measurement of a_s from the world-data including the future proton and deuteron data taken at the EIC [58], we recommend a strict non-singlet analysis at N^{3}LO, for which already now all relevant massless, single- and two-mass corrections are available, cf. Refs. [8, 25, 40, 42, 59, 60], to accomplish a long-standing proposal, cf. Ref. [61], after about 40 years.

Acknowledgments. This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme grant agreement 101019620 (ERC Advanced Grant TOPUP), the UZH Postdoc Grant, grant no. [FK-24-115] and by the Austrian Science Fund (FWF) Grant DOI 10.55776/P33530.

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