Overview of PDF calculations from Lattice QCD

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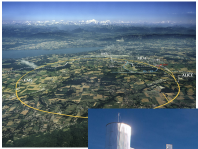
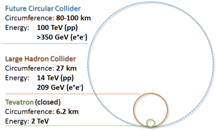
In collaboration with P. Barry (JLAB), L. DelDebbio (Edinburgh), H. Dutrieux (WM), R. Edwards (JLAB), C. Egerer (JLAB), T. Giani (NIKHEF), B. Joo (ORNL), J. Karpie (JLAB), N. Karthik (APS), T. Khan (Brac U.), W. Melnitchouk (JLAB), K. Orginos (College of William & Mary and JLAB), A. Radyushkin (ODU and JLAB), D. Richards (JLAB), E. Romero (JLAB), A. Rothkopf (Stavanger U.), N. Sato (JLAB), R. Sufian (BNL)

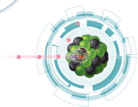
PDFs are of paramount importance because...

- The uncertainties in PDFs are the dominant theoretical uncertainties in Higgs couplings, α_s and the mass of the W boson

- Beyond the LHC, PDFs play an important role, for instance in astroparticle physics, such as for the accurate predictions for signal and background events at ultra–high energy neutrino telescopes (ANITA, IceCube, Pierre Auger Observatory)





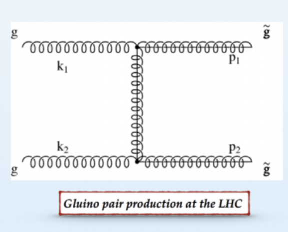


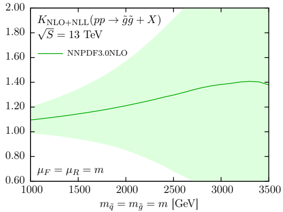
- PDFs will keep playing an important role for any future high energy collider involving hadrons in the initial state. Therefore improving our understanding of PDFs also strengthens the physics potential of such future colliders

Gao, Harland-Lang, Rojo (2018)

PDF uncertainties and BSM Physics

The uncertainty on the PDFs is rapidly becoming one of the limiting factors in searches for new physics.





The relative size of the NLL corrections for gluino pair production was computed.The error in the relative size of the NLL corrections grows very quickly as the gluino mass is increased, mostly as a consequence of the large PDF errors at large values of x. Beenakker et al. (2016)

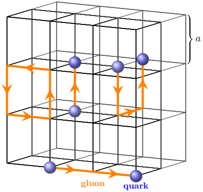
From DIS to PDFs via factorization

- The measurement of PDFs is made possible due to factorization theorems
- Intuitively, factorization theorems tell us that the same universal non-perturbative objects (the PDFs), representing long distance physics, can be combined with many short-distance calculations in QCD to give the cross-sections of various processes (prelude: the LHS could also be from simulated data)

$$\sigma = f \otimes H$$

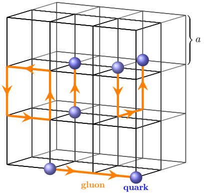
  - f are the PDFs, H is the hard perturbative part and $\otimes$ is convolution.
  - PDFs truly characterize the hadronic target
  - PDFs are essentially non-perturbative

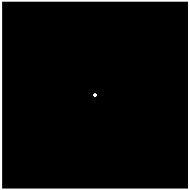
Lattice?



- The natural ab-initio method to study QCD non-perturbatively is on the lattice. But ...
- PDFs are defined as an expectation value of a bilocal operator evaluated along a light-like line.
- Clearly, we can not evaluate this on a Euclidean set-up.

Lattice?





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Global PDF fits

- The first principle calculations are currently being tested and worked out ...
- Usual determination of PDFs is performed by fitting experimental data from several hard scattering cross sections (l-p and p-p collisions).
- Combining the most PDF-sensitive data and the highest precision QCD and EW calculations and employing a statistically robust fitting methodology.
- Need to make sure that new physics effects are not inadvertently fitted away in a PDF fit
- Can achieve high precision for the cases that data are abundant (which is the case for very few distributions) .

Light cone distributions and lattice QCD

Lattice traditionally & global PDF fits

Light cone PDF

$$q(x) = \frac{1}{4\pi} \int_{-\infty}^{\infty} d\omega^- e^{-ixP^+\omega^-} \langle P | \bar{\psi}(\omega^-) W(\omega^-, 0) \gamma^+ \psi(0) | P \rangle$$

where $W(\omega^-, 0) = \mathcal{P} e^{-ig_0 \int_0^{\omega^-} dy^- A^+(y^-)}$

Lattice traditionally & global PDF fits

Light cone PDF

$$\longrightarrow q(x) = \frac{1}{4\pi} \int_{-\infty}^{\infty} d\omega^- e^{-ixP^+\omega^-} \langle P|\bar{\psi}(\omega^-)W(\omega^-,0)\gamma^+\psi(0)|P\rangle$$

Mellin moments $\langle x^k \rangle_q = \int_{-1}^{1} \mathrm{d}x\ x^k\ q(x)$ related to local matrix elements of twist-2 operators

$$\langle P|\bar{\psi}(0)\gamma^{\{\mu_1}D^{\mu_2}...D^{\mu_k\}}\psi(0)|P\rangle = 2\langle x^k \rangle_q (P^{\mu_1}...P^{\mu_k} - \mathrm{traces})$$

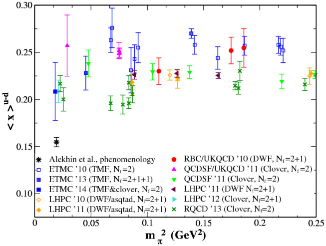
Lattice traditionally & global PDF fits

- Not an issue if every moment were accessible because a probability distribution is completely determined once all its moments are known.
- These studies are limited to the first few (three) moments due to
  - Bad signal to noise ratio
  - Power-divergent mixing on the lattice (discretized space-time does not possess the full rotational symmetry of the continuum).

Lattice traditionally & global PDF fits

Mellin moments

Constantinou (2015)



Lattice traditionally & global PDF fits

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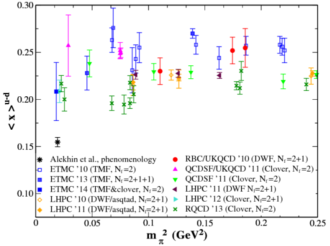

Global fits

- Usual determination of PDFs is performed by fitting experimental data from several hard scattering cross sections (l-p and p-p collisions)
- Combining the most PDF-sensitive data and the highest precision QCD and EW calculations (always assuming that SM holds) and employing a statistically robust fitting methodology
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Lattice traditionally & global PDF fits

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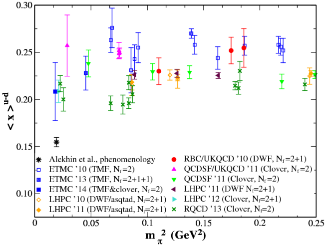
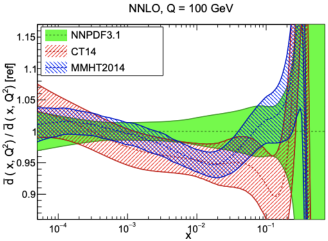


Global fits

Lin et al. (2018)



The Ji Idea

- Lattice QCD computes equal time matrix elements
- Displace quarks in space-like interval
- Boost states to “infinite” momentum
- On the frame of the proton displacement becomes lightlike
- But infinite momentum not possible on the lattice
- Use perturbative matching from finite momentum X. Ji (2013)
- One needs to deal with the divergences

PDFs from the lattice: Pseudo-PDFs Formalism

Starting point: the equal time hadronic matrix element with the quark and anti-quark fields separated by a finite distance Radyushkin (2017)

$$\mathcal{M}^{\alpha}(z,p) \equiv \langle p|\bar{\psi}(0)\,\gamma^{\alpha}\,\hat{E}(0,z;A)\tau_3\psi(z)|p\rangle$$

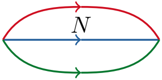
$$\begin{aligned} z &= (0,0,0,z_3) \\ p &= (p^0,0,0,p) \\ \alpha &= 0 \end{aligned}$$

$$\xrightarrow{\text{Lorentz inv.}} \mathcal{M}^{\alpha}(z,p) = 2p^{\alpha}\underbrace{\mathcal{M}_p(-(zp),-z^2)}_{\textbf{Leading twist}} + \cancel{z^{\alpha}\underbrace{\mathcal{M}_z(-(zp),-z^2)}_{\textbf{Higher twist}}}$$

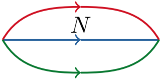
- The Lorentz invariant quantity $\nu = -(zp)$, is the "Ioffe time"
- Ioffe time PDFs $\mathcal{M}(\nu, z_3^2)$ defined at a scale $\mu^2 = 4e^{-2\gamma_E}/z_3^2$ (at leading log level) are the Fourier transform of regular PDFs $f(x,\mu^2)$ Balitsky, Braun (1988), Braun et al. (1995)

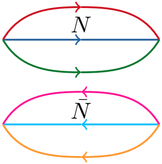
$$\mathcal{M}(\nu, z_3^2) = \int_{-1}^{1} dx\, f(x, 1/z_3^2) e^{ix\nu}$$

Signal to Noise

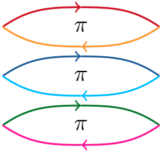


$$\langle C_N(t)\rangle \sim e^{-m_N t}$$





$$\langle |C_N(t)|^2\rangle \sim e^{-3m_\pi t}$$



Statistical accuracy drops exponentially with increasing momentum P

$$\mathrm{StN}(O) = \frac{\langle O\rangle}{\sqrt{\mathrm{var}(O)}} \propto e^{-[E_N(P)-3/2m_\pi]t}$$

G. Parisi (1984) P. Lepage (1989) Statistical accuracy drops exponentially with the increasing momentum limiting the maximum achievable momentum.

Obtaining the Ioffe time PDF

$$z_3 \to 0 \Rightarrow \mathcal{M}_p(\nu, z_3^2) = \mathcal{M}(\nu, z_3^2) + \mathcal{O}(z_3^2)$$

But.... large $\mathcal{O}(z_3^2)$ corrections prohibit the extraction.

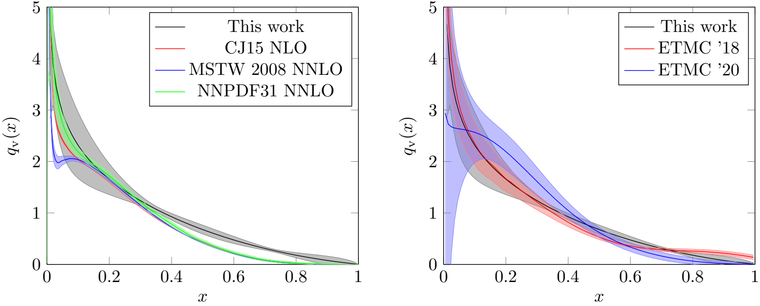
In a ratio z_3^2 corrections might cancel Radyushkin (2017)

$$\mathfrak{M}(\nu, z_3^2) \equiv \frac{\mathcal{M}_p(\nu, z_3^2)}{\mathcal{M}_p(0, z_3^2)}$$

- Much smaller $\mathcal{O}(z_3^2)$ corrections and therefore this ratio could be used to extract the Ioffe time PDFs
- All UV singularities are exactly cancelled and when computed in lattice QCD it can be extrapolated to the continuum limit
- $$\mathfrak{M}(\nu, z^2) = \int_0^1 d\alpha\, \mathcal{C}(\alpha, z^2\mu^2, \alpha_s(\mu))\,\mathcal{Q}(\alpha\nu, \mu) \; + \sum_{k=1}^{\infty} \mathcal{B}_k(\nu)(z^2)^k \,,$$

  μ is the factorization scale and $\mathcal{Q}(\nu, \mu)$ is the Ioffe time PDF

Results with $N_f = 2+1$ fermions for the nucleon with physical pion masses



Our determinination of the phys. pion mass nucleon valence PDF compared to pheno and other lattice determinations. Joo, Karpie, Orginos, Radyushkin, Richards, S.Z. Phys.Rev.Lett. 125 (2020) 23, 232003

Challenges

- Physical pion mass
- Finite Volume effects
- Continuum limit (cut off effects)
- Excited state contamination
- Large momentum-Signal to noise ratio (critical slowing down, topological freezing, large autocorrelations)
- Higher twist effects
- perturbative uncertainties (matching, Wilson coefficients)
- handling of the inverse problem UBIQUITOUS AND UNAVOIDABLE

The pertinent systematics in PDF extraction

- Parton distribution functions or distribution amplitudes may be defined in lattice QCD by inverting the quasi-Fourier transform of a certain class of hadronic position-space matrix elements
- One example are the Ioffe-time PDFs, $\mathfrak{M}_R$, related to the physical PDF $q_v(x, \mu^2)$ via the integral relation

$$\mathfrak{M}_R(\nu, \mu^2) \equiv \int_0^1 dx \, \cos(\nu x) \; q_v(x, \mu^2)$$

Karpie, Orginos, Rothkopf, S.Z. JHEP 1904 (2019) 057

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Only a handful of lattice data

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Cosine not orthogonal in $[0, 1]$

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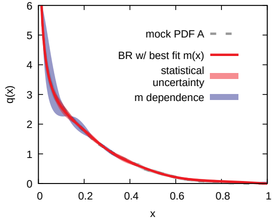
Cosine not orthogonal in $[\mathbf{0},\mathbf{1}]$

- The task at hand is then to reconstruct the PDF $q_v(x,\mu^2)$ given a limited set of simulated data for $\mathfrak{M}_R(\nu,\mu^2)$.
- The extraction is highly ill-posed, so one has to resort to regularization strategies in order to find a way to reliably estimate the PDF from the data at hand

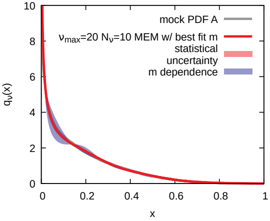
Karpie, Orginos, Rothkopf, S.Z. JHEP 1904 (2019) 057

Advanced PDF Reconstructions

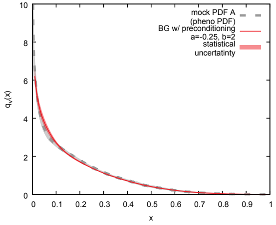
Bayesian Reconstruction



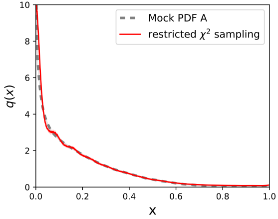
Max. Entropy Method



Backus-Gilbert algorithm

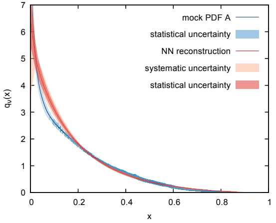


HMC χ^2 evaluation



- Bayesian Reconstruction
- Max. Entropy Method
- Backus-Gilbert algorithm
- HMC χ^2 evaluation
- Neural Network

Neural Network



The Continuum and Leading Twist Limits of Parton Distribution Functions in Lattice QCD

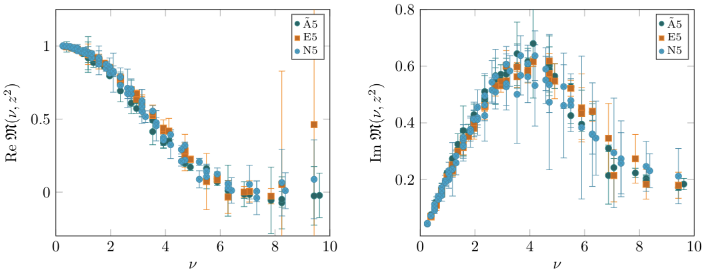
- continuum limit
- higher twist effects
- employing Jacobi polynomials
- excited state contamination & summation Generalized Eigenvalue Problem (sGEVP)
- Karpie, Orginos, Radyushkin and S.Z. JHEP 11 (2021) 024

The Continuum and Leading Twist Limits of Parton Distribution Functions in Lattice QCD

ID	a(fm)	M_π(MeV)	β	c_{SW}	κ	$L^3 \times T$	N_{cfg}
$\widetilde{A}5$	0.0749(8)	446(1)	5.2	2.01715	0.13585	$32^3 \times 64$	1904
E5	0.0652(6)	440(5)	5.3	1.90952	0.13625	$32^3 \times 64$	999
N5	0.0483(4)	443(4)	5.5	1.75150	0.13660	$48^3 \times 96$	477

Parameters for the lattices generated by the CLS collaboration using two flavors of $\mathcal{O}(a)$ improved Wilson fermions.

The Continuum and Leading Twist Limits of Parton Distribution Functions in Lattice QCD



The real (LHS) and the imaginary (RHS) part of the reduced ITDs of the three lattice ensembles used in this study. We see that for the range of Ioffe times that is covered by our data the three ensembles have a pretty good overlap. The statistical and systematic errors are added in quadrature.

The Continuum and Leading Twist Limits of Parton Distribution Functions in Lattice QCD

A Taylor expansion in lattice spacing gives the continuum reduced pseudo-ITD $\mathfrak{M}_{\rm cont}$ and lattice spacing corrections

$$\mathfrak{M}(p,z,a) = \mathfrak{M}_{\rm cont}(\nu, z^2) + \sum_{n=1} \left(\frac{a}{|z|}\right)^n P_n(\nu) + (a\Lambda_{\rm QCD})^n R_n(\nu)$$

With an $O(a)$ improved lattice action, the lattice spacing errors related to the momentum p, must come in from the momentum transfer. This feature is known in the improvement of the local vector current. The higher twist power corrections are added as nuisance terms similar to the lattice spacing terms. The functional form is given by

$$\mathfrak{M}_{\rm cont}(\nu, z^2) = \mathfrak{M}_{\rm lt}(\nu, z^2) + \sum_{n=1} (z^2\Lambda^2_{\rm QCD})^n B_n(\nu)\,.$$

The Continuum and Leading Twist Limits of Parton Distribution Functions in Lattice QCD

All of the unknown functions, $q_-(x)$, $q_+(x)$, $P_1(\nu)$, $R_1(\nu)$, and $B_1(\nu)$, are parameterized using Jacobi polynomials.
The Jacobi polynomials, $j_n^{(\alpha,\beta)}(z)$, are defined in the interval $[-1,1]$ and they satisfy the orthogonality relation

$$\int_{-1}^{1} dz(1-z)^\alpha(1+z)^\beta j_n^{(\alpha,\beta)}(z) j_m^{(\alpha,\beta)}(z) = \tilde{N}_n^{(\alpha,\beta)}\delta_{n,m} \,,$$

for $\alpha, \beta > -1$. COV $x = \frac{1-z}{2}$ or $z = 1-2x$. This transformation maps the interval $[-1,1]$ to the interval $[0,1]$ and the orthogonality weight becomes $(1-z)^\alpha(1+z)^\beta = 2^{\alpha+\beta}x^\alpha(1-x)^\beta$. We then introduce the transformed Jacobi polynomials $J_n^{(\alpha,\beta)}(x)$, as

$$J_n^{(\alpha,\beta)}(x) = \sum_{j=0}^{n} \omega_{n,j}^{(\alpha,\beta)} x^j \,.$$

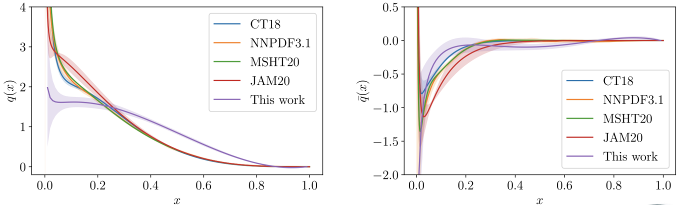
The Continuum and Leading Twist Limits of PDFs

Since the Jacobi polynomials form a complete basis of functions in the interval of [0,1], the PDFs can be written as

$$q_{\pm}(x) = x^{\alpha}(1-x)^{\beta} \sum_{n=0}^{\infty} {}_{\pm}d_n^{(\alpha,\beta)} J_n^{(\alpha,\beta)}(x)$$

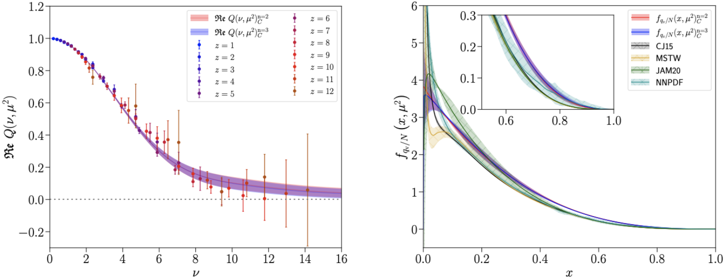
for any α and β. The choice of those parameters does affect the convergence of the coefficients ${}_{\pm}d_n^{(\alpha,\beta)}$. One needs to truncate the series introducing in this way some model dependence which can be easily controlled. The control of the truncation can be improved if one fits for the optimal values of α and β for that given order of truncation. In other words, the rate of convergence of the series can be optimized by tuning the values of α and β.

The Continuum and Leading Twist Limits of PDFs



Isovector quark and anti-quark distributions-comparing to phenomenology

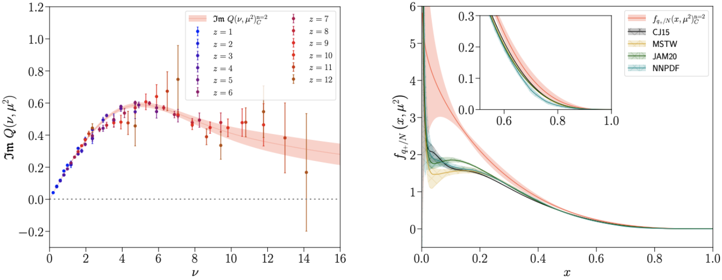
Towards High-Precision Parton Distributions From Lattice QCD via Distillation



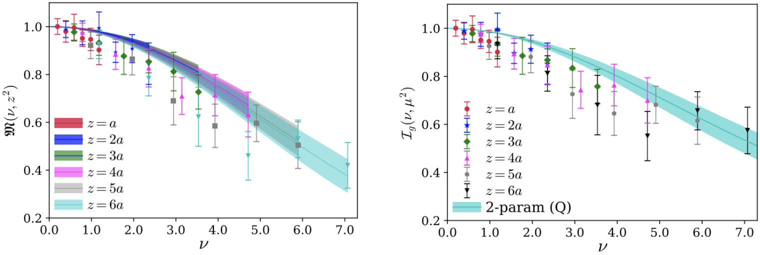
The real component of the matched ITD at $\mu = 2$ GeV in $\overline{\text{MS}}$ fit by cosine transforms of two- and three-parameter model PDFs. The nucleon unpolarized valence quark PDF at 2 GeV in $\overline{\text{MS}}$ determined from the uncorrelated cosine transform fits applied to real component of the matched ITD. Comparisons are made with the NLO global analyses of CJ15 and JAM20, and the NNLO analyses of MSTW and NNPDF at the same scale.

Egerer, Edwards, Kallidonis, Orginos, Radyushkin, Richards, Romero and S.Z. JHEP11(2021)148

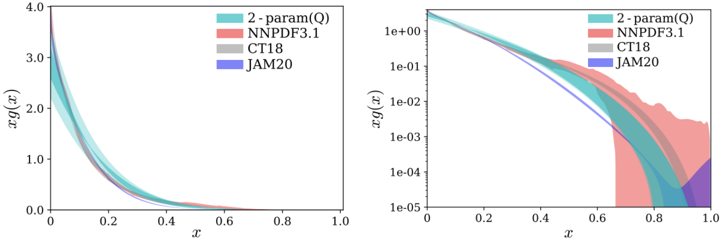
Towards High-Precision Parton Distributions From Lattice QCD via Distillation



The imaginary component of the matched ITD at $\mu = 2$ GeV in $\overline{\text{MS}}$ fit by the sine transform of a two-parameter model PDF. Data has been fit for $z/a \leq 12$, and correlations have been neglected. The nucleon unpolarized plus quark PDF at 2 GeV in $\overline{\text{MS}}$ determined from the uncorrelated sine transform fits applied to the imaginary component of the matched ITD. Comparisons are made with the NLO global analyses of CJ15 and JAM20, and the NNLO analyses of MSTW and NNPDF at the same scale. Egerer, Edwards, Kallidonis, Orginos, Radyushkin, Richards, Romero and S.Z. JHEP11(2021)148

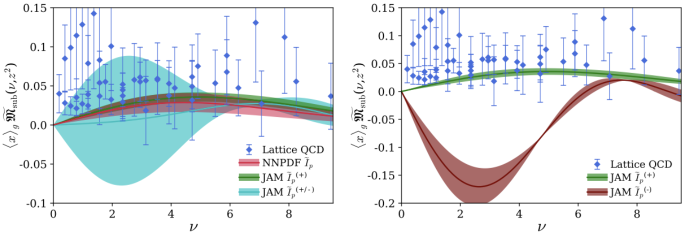


Khan, Sufian, Karpie, Monahan, Egerer, Joo, Morris, Orginos, Radyushkin, Richards, Romero and S.Z. Phys.Rev.D 104 (2021) 9, 094516 Lattice reduced pseudo-ITD shown along with their reconstructed fitted bands and the $\overline{\mathrm{MS}}$ matched ITD at 2GeV.



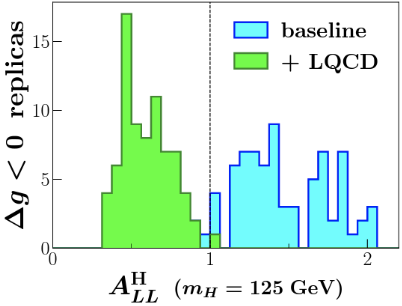
Khan, Sufian, Karpie, Monahan, Egerer, Joo, Morris, Orginos, Radyushkin, Richards, Romero and S.Z. Phys.Rev.D 104 (2021) 9, 094516 Unpolarized gluon PDF (cyan band) extracted from our lattice data using the 2-param (Q) model. We compare our results to gluon PDFs extracted from global fits to experimental data, CT18, NNPDF3.1, and JAM20. Normalization of the gluon PDF using the gluon momentum fraction $\langle x\rangle_g^{\overline{MS}}(\mu = 2\,\mathrm{GeV})$=0.427(92) from Alexandrou et al Phys.Rev.D 101 (2020) 9, 094513 . On the L/RHS the same distributions with different scales for $x\,g(x)$ to enhance the view of the large-x region.

Gluon helicity distribution



Egerer, Joo, Karpie, Karthik, Khan, Monahan, Morris, Orginos, Radyushkin, Richards, Romero, Sufian and S.Z, Phys.Rev.D 106 (2022) 9, 094511 De Florian, Forte and Vogelsang Phys. Rev. D 109, 074007 JAM Collaboration N.T. Hunt-Smith et al 2403.08117 [hep-ph] The lattice reduced pITD and the gluon helicity ITD constructed from global fits. In the LHS the red band denotes the ITD constructed from the gluon helicity distribution by the NNPDF collaboration. The green band and the cyan band represent the gluon helicity ITD determined by the JAM collaboration with and without the positivity constraint. The green band and the maroon band represent the gluon helicity ITD determined by the JAM collaboration associated with the positive and negative gluon helicity PDF solutions.

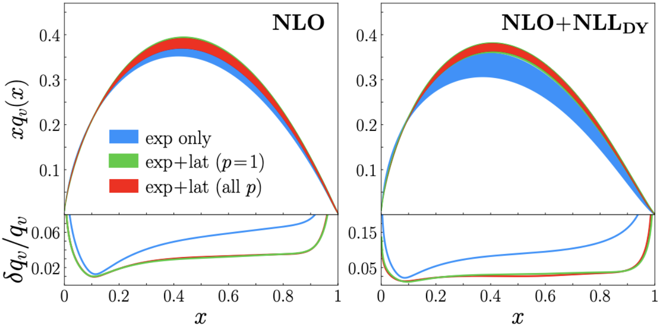
Gluon helicity distribution



JAM Collaboration N.T. Hunt-Smith et al 2403.08117 [hep-ph]

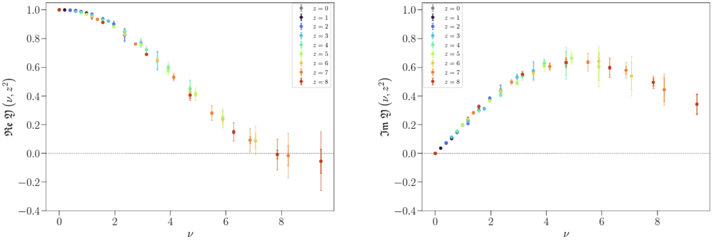
Lattice data added to the "baseline" don't lead to negative cross-sections for physical Higgs mass, so still one can not exclude them. Finally, the combination of baseline, lqcd data and high-x polarized DIS data resolved the debate.

Complementarity of experimental and lattice QCD data on pion parton distributions



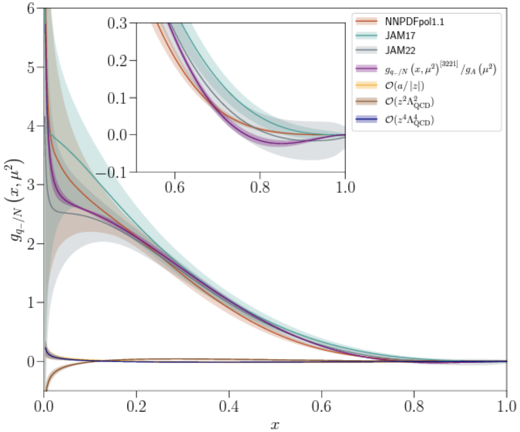
Valence quark distributions (**top**) when extracted from experimental data alone (blue), combined with the $p = 1$ lattice data (green), and combined with all the lattice data (red) for the NLO (**left**) and NLO+NLL$_{\mathrm{DY}}$ (**right**) cases, along with the relative uncertainties (**bottom**). The bands represent a 1σ uncertainty level. Barry, Egerer, Karpie, Melnitchouk, Orginos, Richards, Sato, Sufian, Qiu, S.Z. Phys.Rev.D 105 (2022) 11, 114051

Helicity PDF



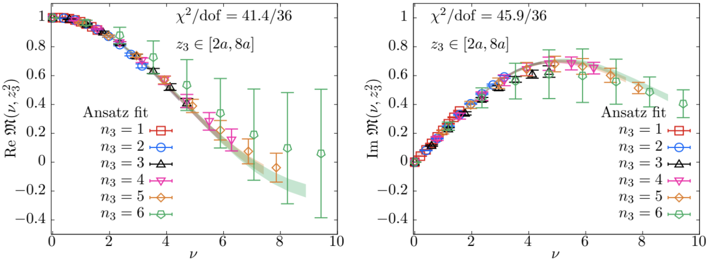
Edwards,Egerer, Karpie, Karthik, Monahan, Morris, Orginos, Radyushkin, Romero, Sufian and S.Z. JHEP 03 (2023) 086

Real and Imaginary components of the reduced pseudo-ITD



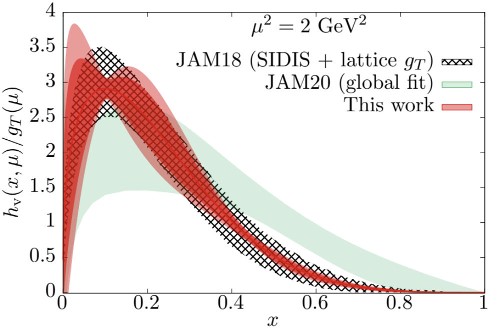
Edwards, Egerer, Karpie, Karthik, Morris, Orginos, Radyushkin, Romero, Sufian and S.Z. Phys.Rev.D 105 (2022) 3, 034507 The leading-twist valence helicity quark PDF (purple) and x-space contaminations compared with the recent global analyses

Transversity PDF



Egerer, Kallidonis, Karpie, Karthik, Morris, Orginos, Radyushkin, Romero, Sufian and S.Z. Phys.Rev.D 105 (2022) 3, 034507 Reconstruction of transversity PDF based on a "Jam Ansatz". The real and imaginary parts of $\mathfrak{M}$ are shown as a function of ν. They show the best fit bands resulting from an analysis assuming the PDF ansatz. The fits shown in the figure incorporated the data points at all momenta with $z_3 \in [2a, 8a]$. The color of the bands and the data points distinguish the fixed value of momenta $P_3 = 0.41 n_3$ GeV used.

Transversity PDF



Egerer, Kallidonis, Karpie, Karthik, Morris, Orginos, Radyushkin, Romero, Sufian and S.Z. Phys.Rev.D 105 (2022) 3, 034507 The valence transversity distribution $h_{\mathrm{v}}(x,\mu)/g_T(\mu)$. The inner red band includes only the statistical error and the outer red band includes statistical and systematical errors in the PDF reconstruction. Comparison is made with the previous phenomenological determinations using SIDIS and lattice g_T (JAM18), shown using a patterned band, and with the recently updated global fit analysis (JAM20) of the single transverse spin asymmetry data (but, without including lattice g_T), shown as a green band.

Conclusions and outlook

- PDFs are needed as theoretical inputs to all hadron scattering experiments and in some cases are the largest theory uncertainty.
- The lattice community is by now able to provide ab-initio determinations of PDFs without theoretical obstructions.
- The interplay between lattice QCD and global fits is very important
- Also important in the search of New Physics Gao, Harland-Lang, Rojo (2018)
- What next?
- **Many thanks for your attention!!!**