Lattice theory for Hot and Cold QCD

Martha Constantinou

Temple University

2022 NSAC Long-Range Plan
Town Hall Meeting
on Hot and Cold QCD

September 23, 2022

★ Lattice QCD broad program, many successes and potential is an integral part of the 2015 NCAS Long Range Plan:

- ⇨ QCD and the Structure of Hadrons and Nuclei
- ⇨ QCD and the Phases of Strongly Interacting Matter
- ⇨ Understanding the Glue That Binds Us All
- ⇨ Nuclear Structure and Reactions
- ⇨ Fundamental Symmetries and Neutrinos
- ⇨ Theoretical / Computational Nuclear Physics
- ⇨ Facilities and Tools
- ⇨ Broader Impacts

★ The advances of lattice QCD in the last 7 years have been impressive

- ⇨ calculations at physical quark masses
- ⇨ precision calculations with controlled systematics (discretization, volume, excited states,...)

★ The field has great momentum and will be impactful to the cold & hot QCD community

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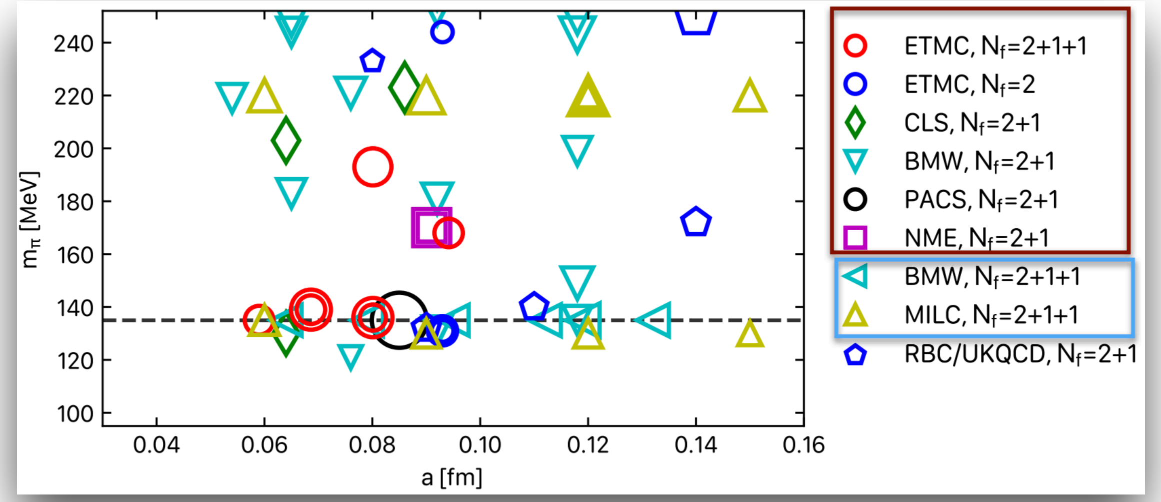

[Finkenrath, plenary talk, Lattice 2022]

Simulations for hadron structure and beyond

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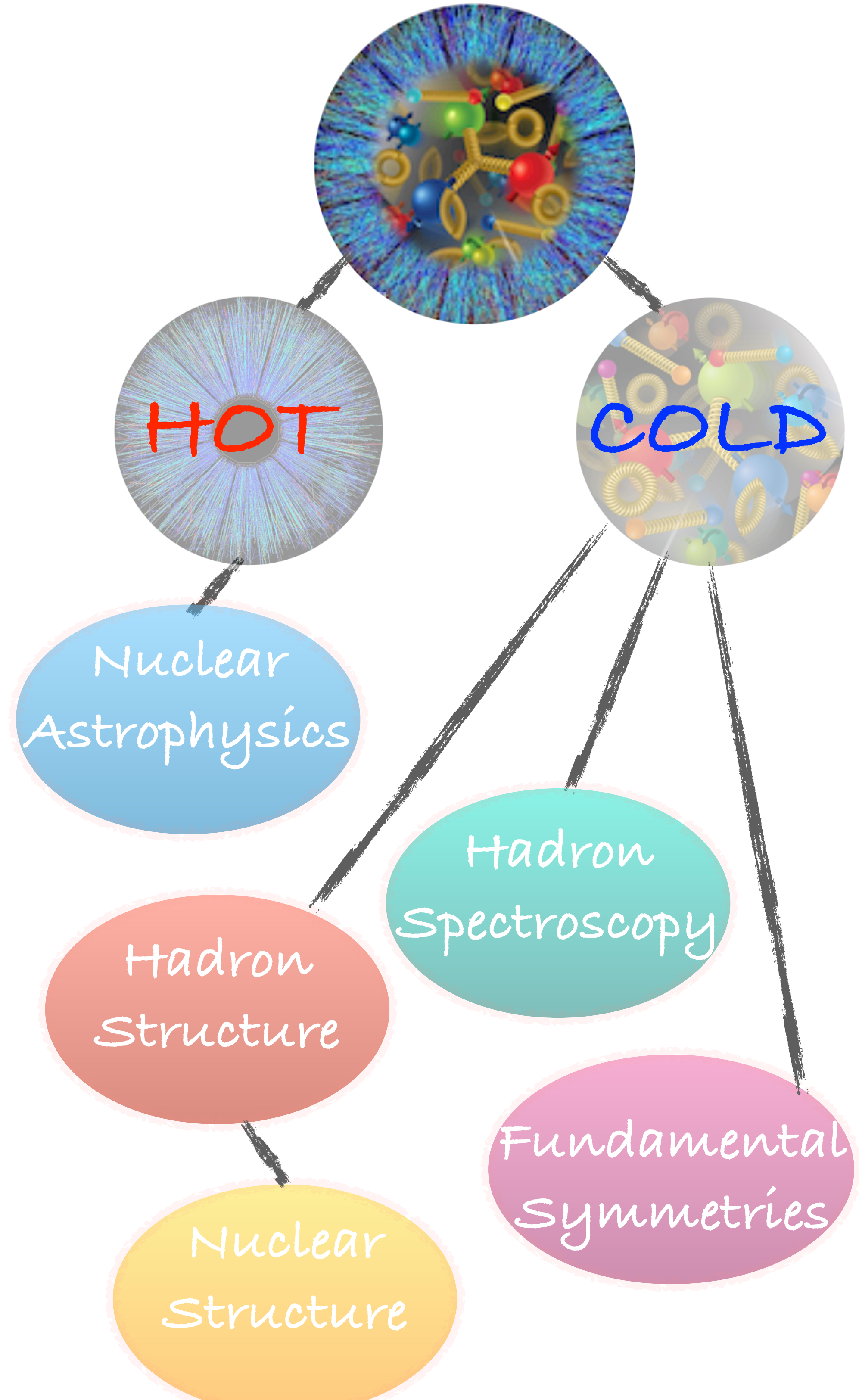
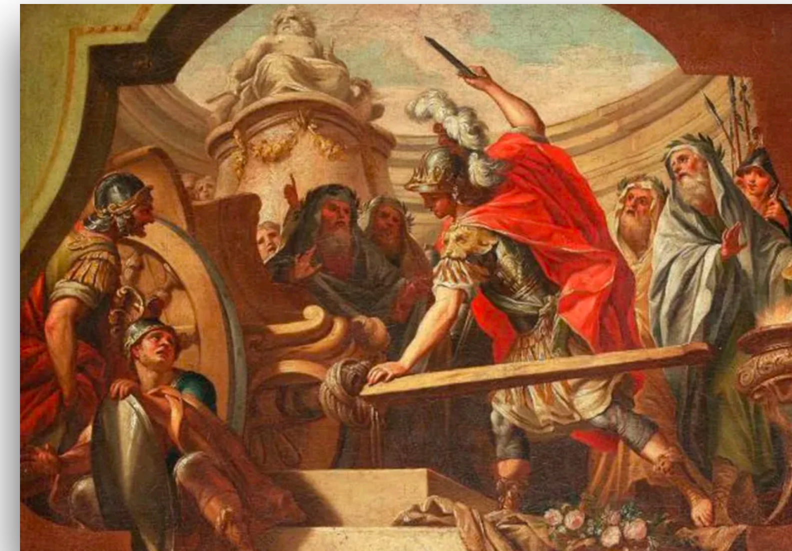
USQCD Nuclear Physics Program

★ Important Lattice QCD contributions that complement the experimental program in both Hot and Cold QCD



In the quest of solving complex problems



“Οτι δεν λύνεται, κόβεται”

Alexander the Great while cutting the Gordian knot

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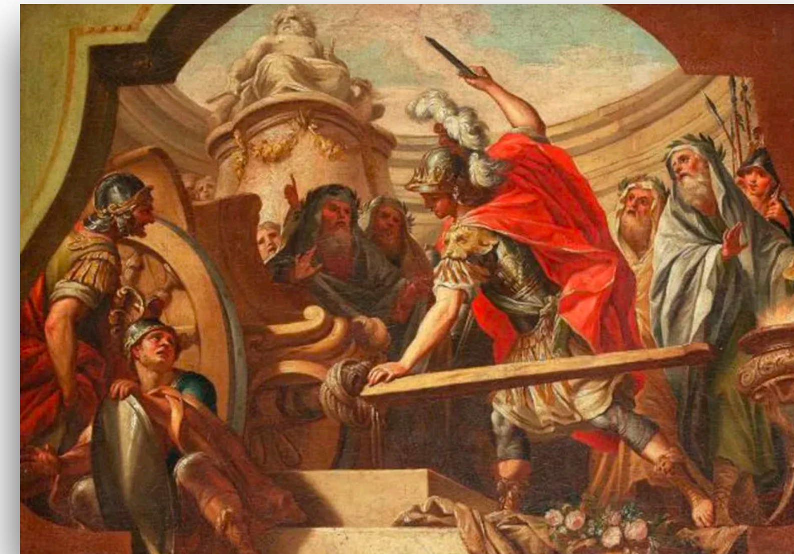
$$\mathscr{L}_{\rm QCD} = \sum_f \bar{\psi}_f \left(i\gamma^\mu D_\mu - m_f \right) \psi_f - \frac{1}{4} F^a_{\mu\nu} F^{a\,\mu\nu}$$



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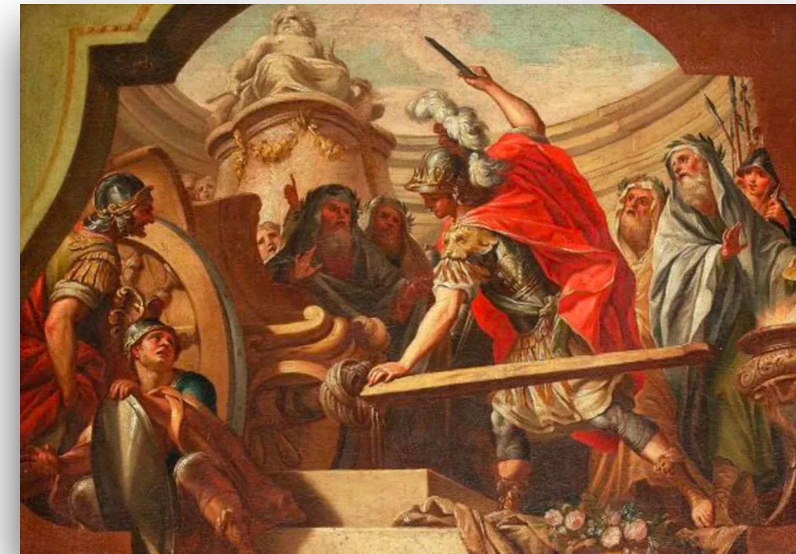

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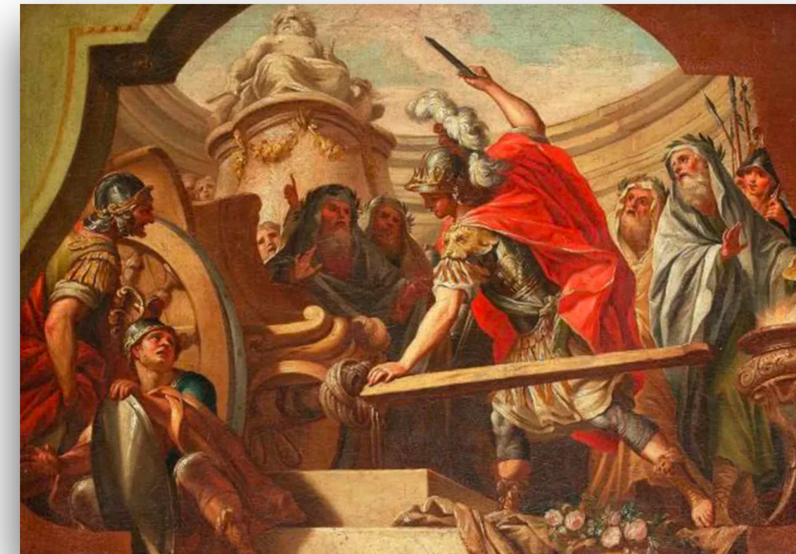

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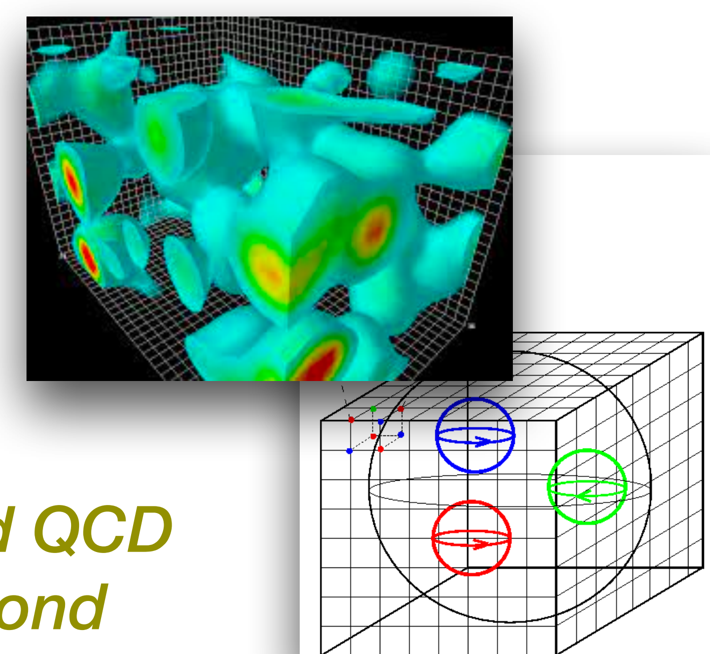
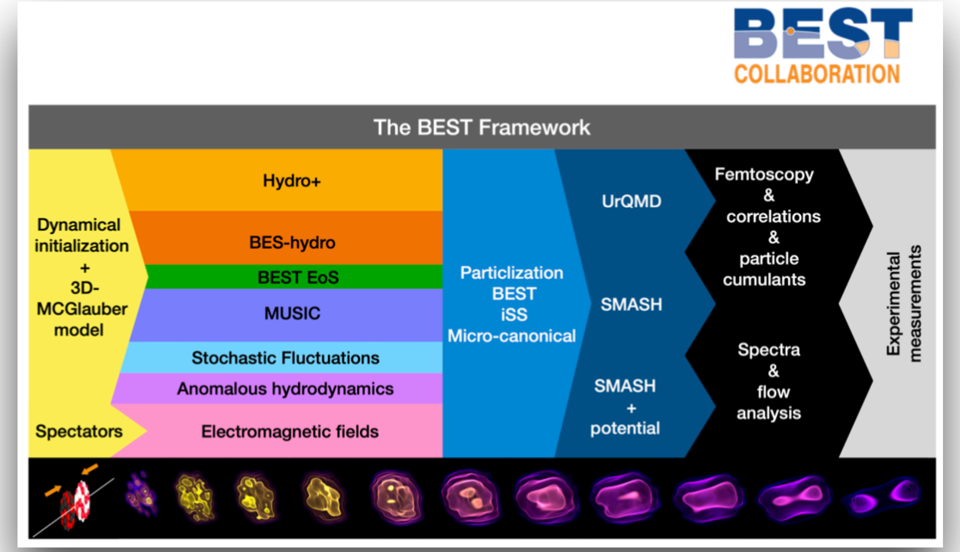
Hot & Cold QCD and beyond

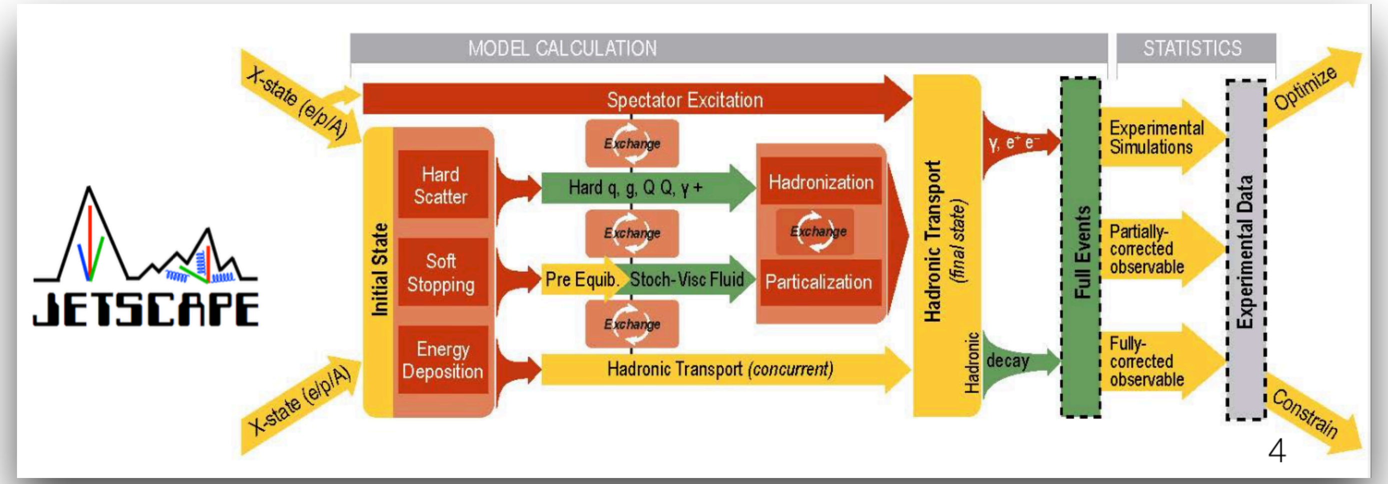


HOT & Dense QCD Matter

- ⇨ heavy-quark energy loss and diffusion constant
- ⇨ bottomonia properties in QGP
- ⇨ Critical point in QCD phase diagram
- ⇨ QCD equation of state ($\mu_B > 0$)
- ⇨ and many more

input to experimental and theoretical investigations





- Discover / put constraints on critical point in nuclear phase diagram
- Locate the onset of chiral symmetry restoration by observing correlations related to anomalous hydrodynamic effects in QGP

Study of QGP:

- Interpretation of jet measurements via numerical modeling and simulation
- Comparison of theory calculations with experimental data with advanced statistical tools

Heavy quark diffusion constant

P. Petreczky, Fri 4:00 pm

★ What is the thermalization rate of heavy quarks in QGP?
(energy loss → heavy quark diffusion coefficient)

★ Perturbative expansion fails → first-principle calculations required

★ First results for full QCD appeared recently!
(gradient-flowed color-electric correlators)

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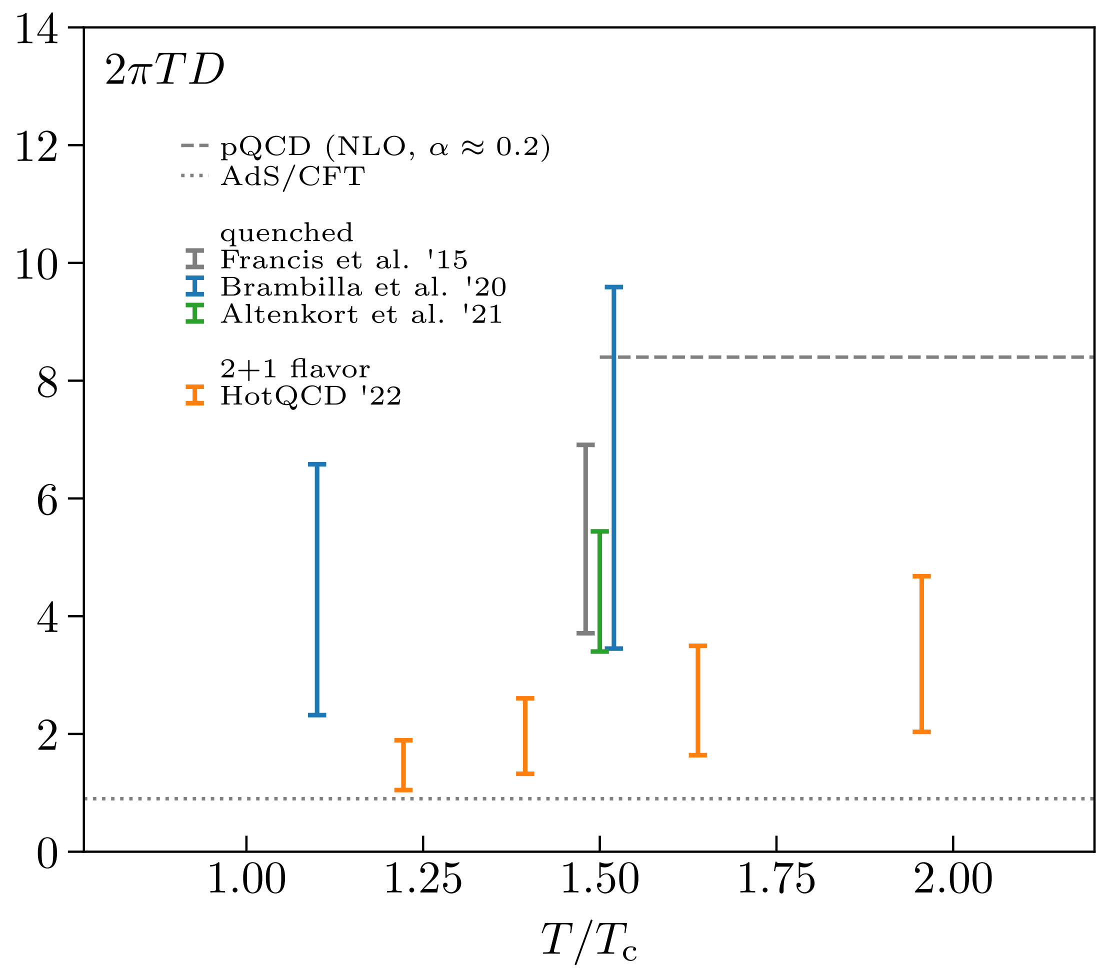

[Luis Altenkort *et al.*, Quark Matter 2022]

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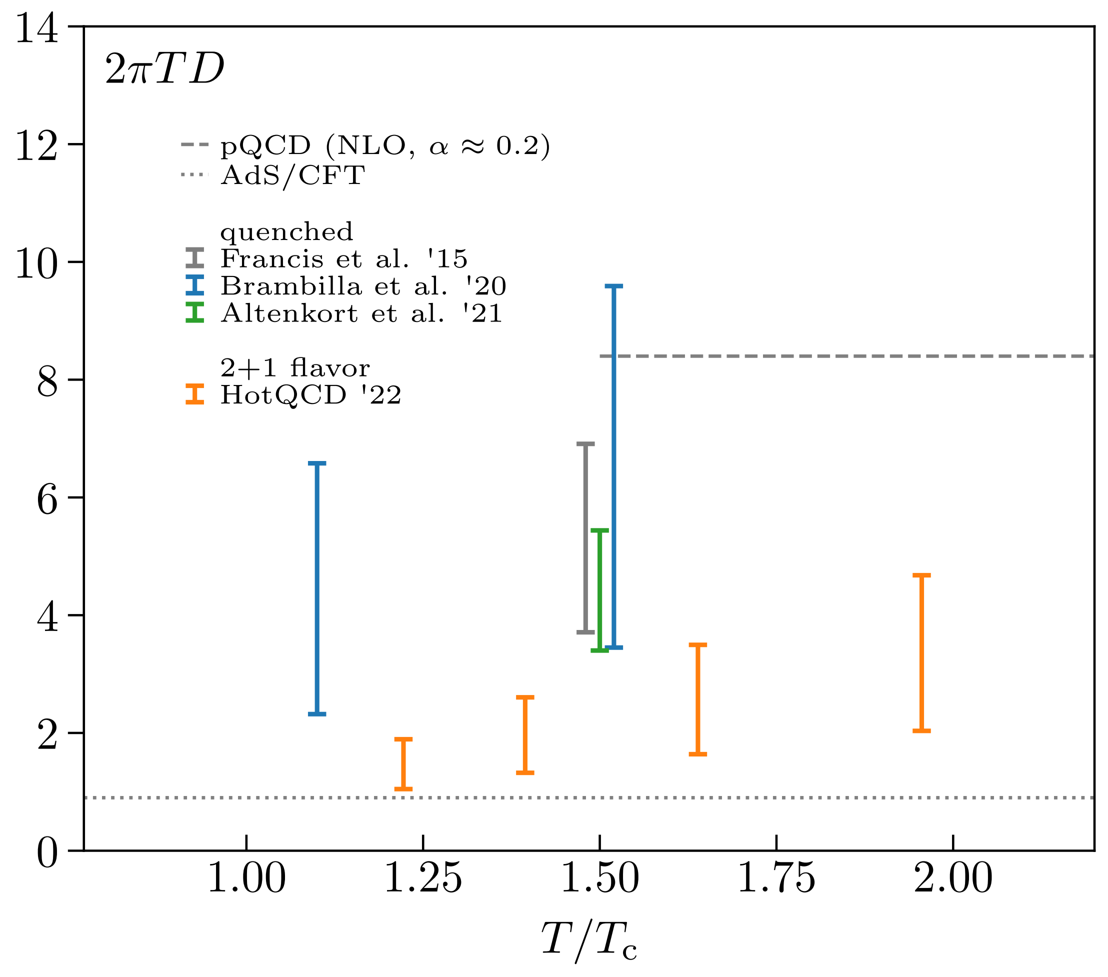
- ★ 2+1 flavor data closer to the predictions of AdS/CFT and indicate a faster loss of energy
- ★ Relevant to ongoing and upcoming heavy-ion collisions experiments (sPHENIX, STAR) and LHC



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QCD equation of state

for hydrodynamic modeling of heavy-ion collisions

C. Ratti, Sat 8:50 am

★ Finite baryon density: Taylor expansion for leading μ_B derivatives of observables

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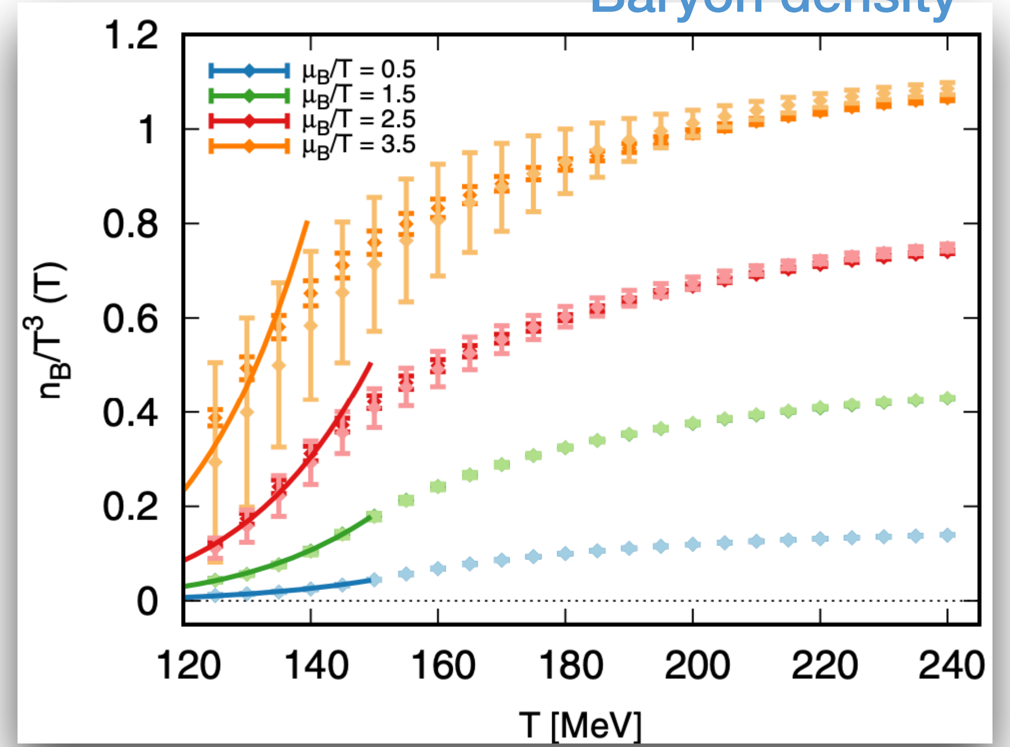
- ★ Novel summation scheme for the QCD EoS at finite μ_B
  - ⇨ improved convergence properties compared to Taylor expansion
  - ⇨ high baryonic chemical potentials

Baryon density



[Borsányi et al., PRL 126, 232001 (2021)]

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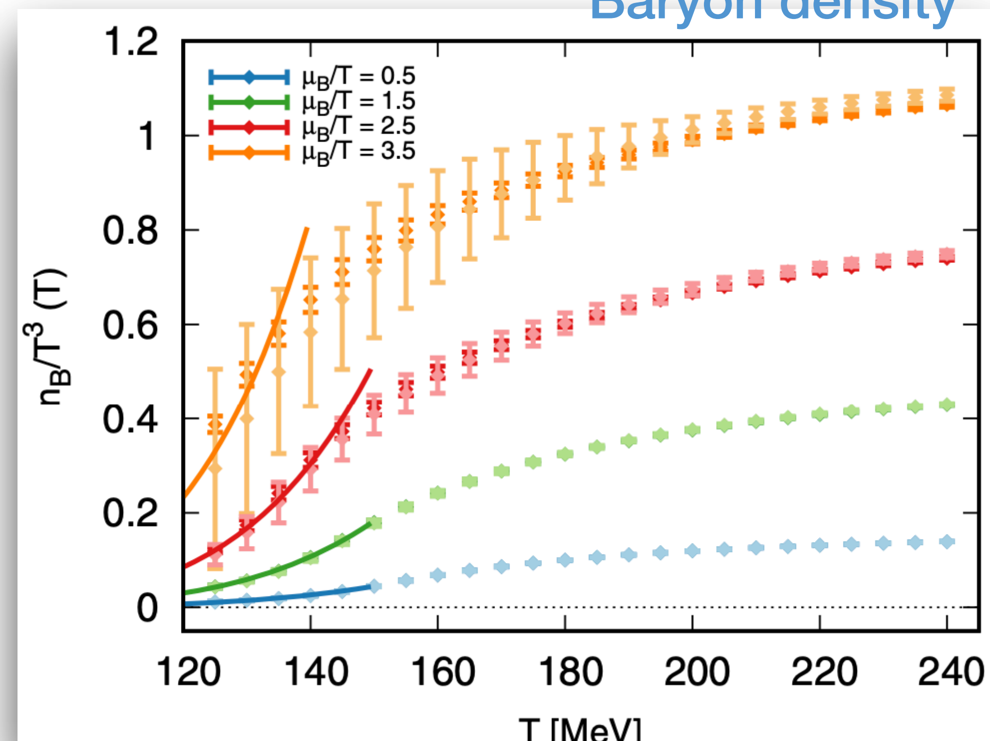

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★ Huge implications on the QCD phase diagram

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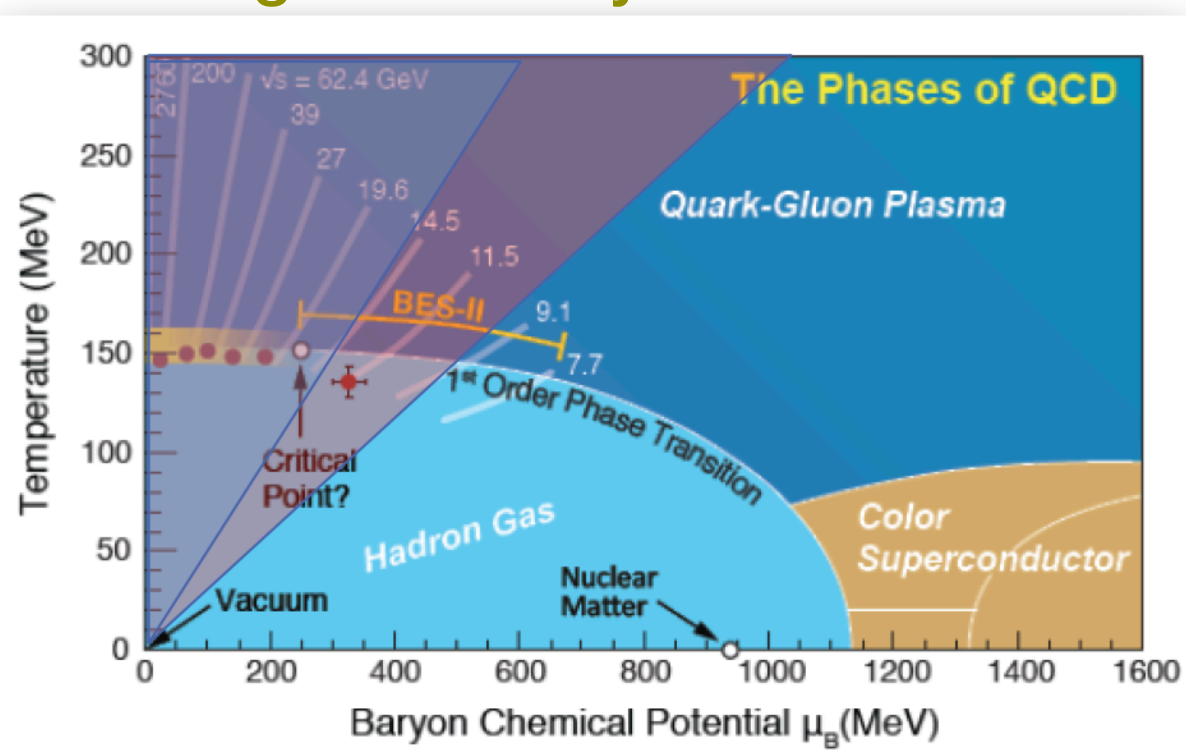

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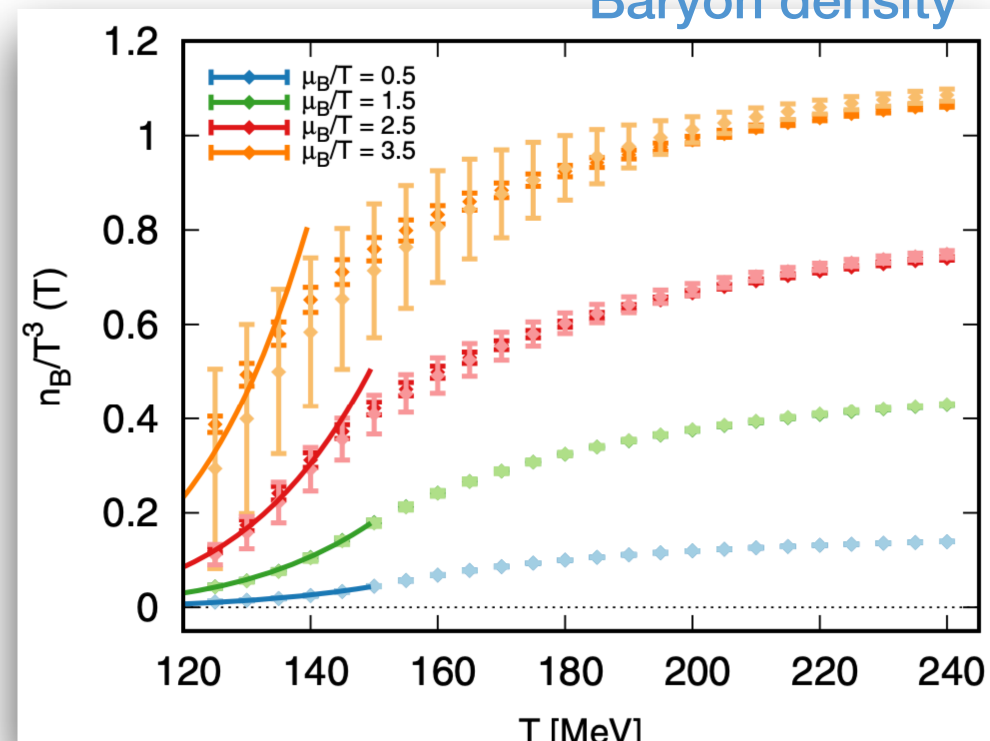

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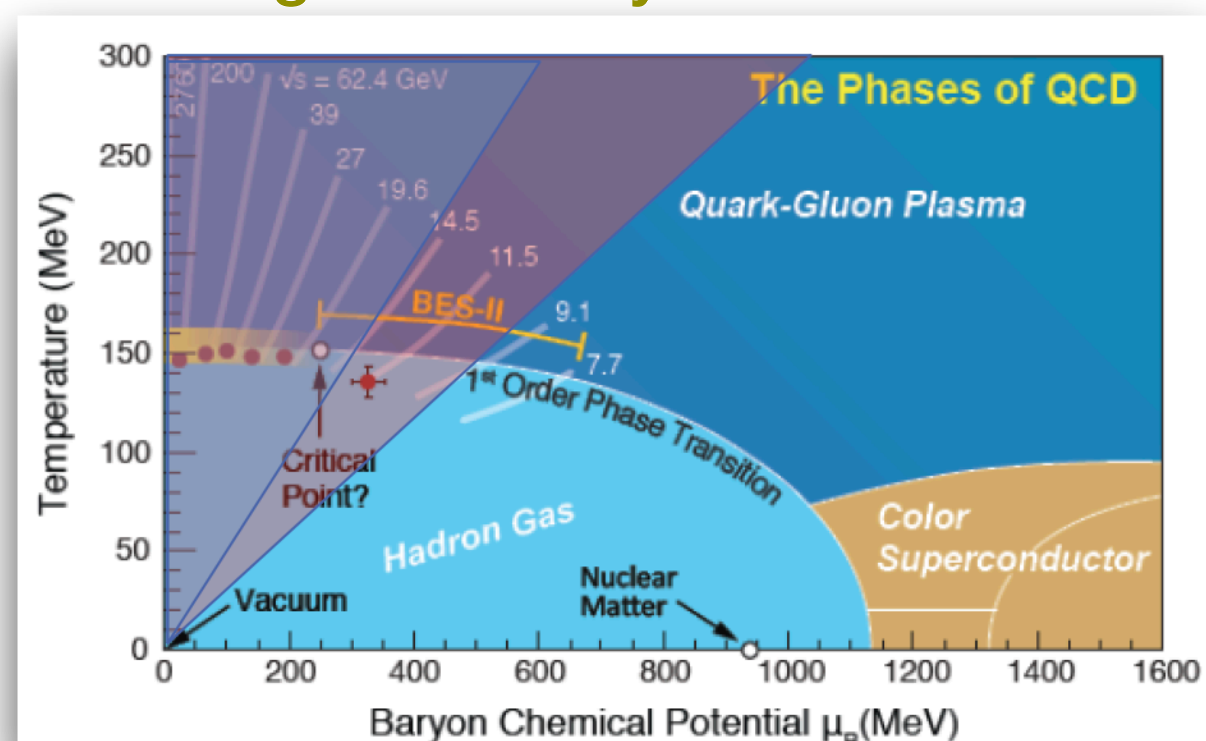


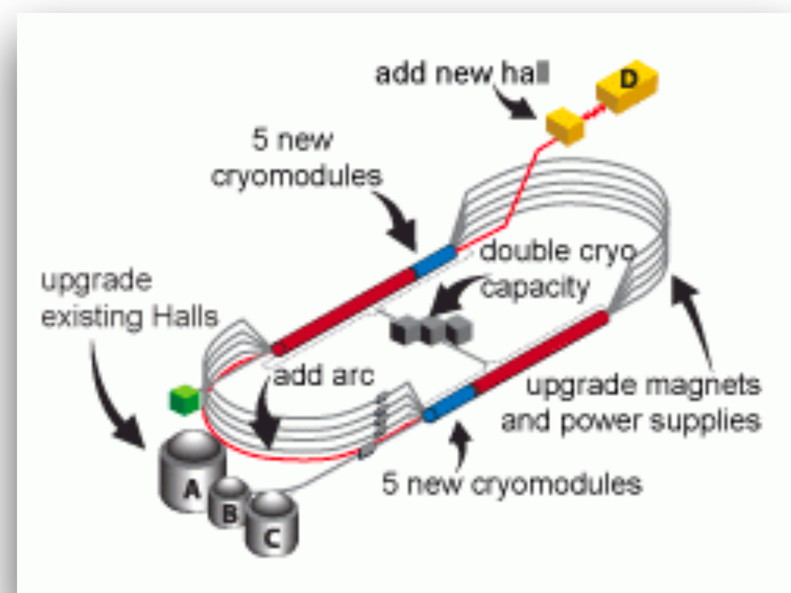
Relevant to experimental program

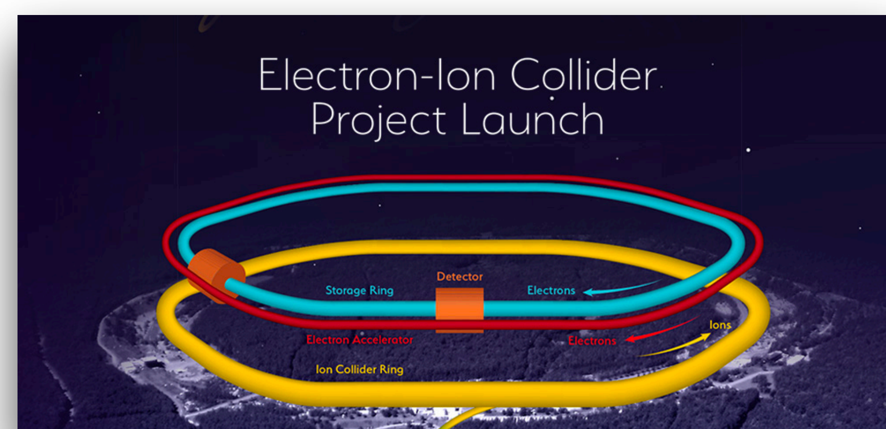
(RHIC BES-II, NA61/SHINE, HADES, CBM)

COLD QCD

- Coupled-channel scattering amplitudes
- Three-body decays
- Proton spin and mass decomposition
- Gluonic structure of hadrons
- Connection between QCD and nuclear physics
- and many more

Complement experiments and coordinated theoretical efforts





TMD Collaboration

U.S. DEPARTMENT OF ENERGY | Office of Science

Hadron Spectroscopy

J. Dudek, Sat 8:50 am

★ Remarkable progress in several directions:
- ⇨ baryon and meson states
- ⇨ Scattering amplitudes in finite volume
- ⇨ exotic decays / three-body decays

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to the infinite volume scattering amplitudes determined in experiments

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★ Formalism extended to multi-channel scattering

★ Reliable extraction of coupled-channel scattering amplitudes at the forefront of field:

extraction of phase shifts and resonances

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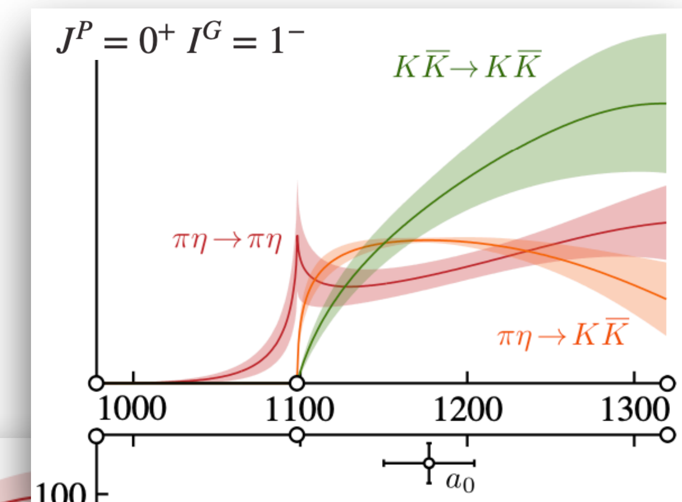
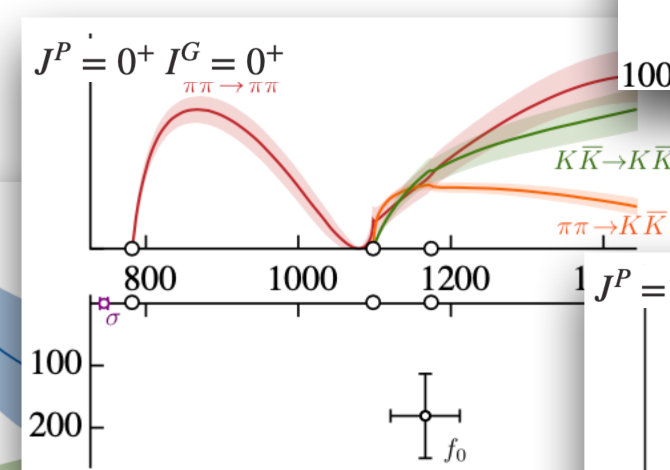
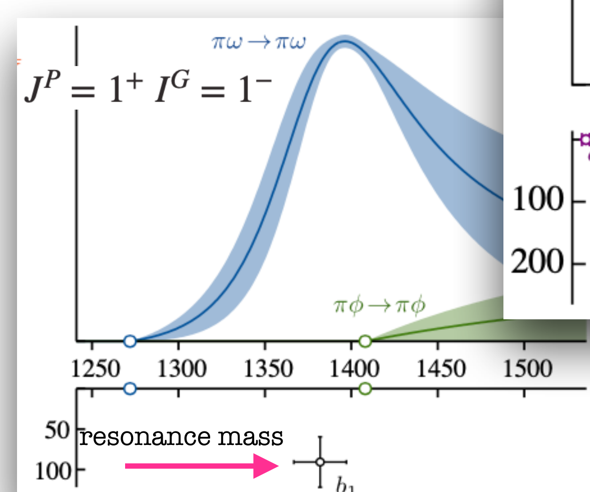


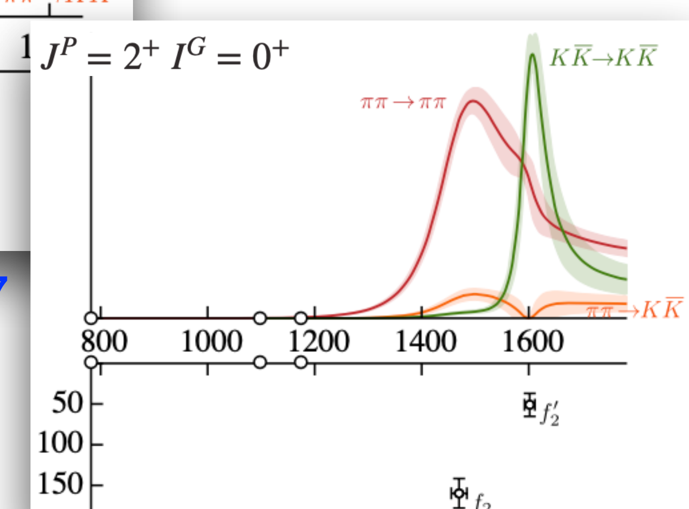
[Dudek et al., PRD 93 094506 (2016)]



[Briceño et al., PRD 97 054513 (2018)]



[Woss et al., PRD 100 054506 (2019)]



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Hadron Spectroscopy

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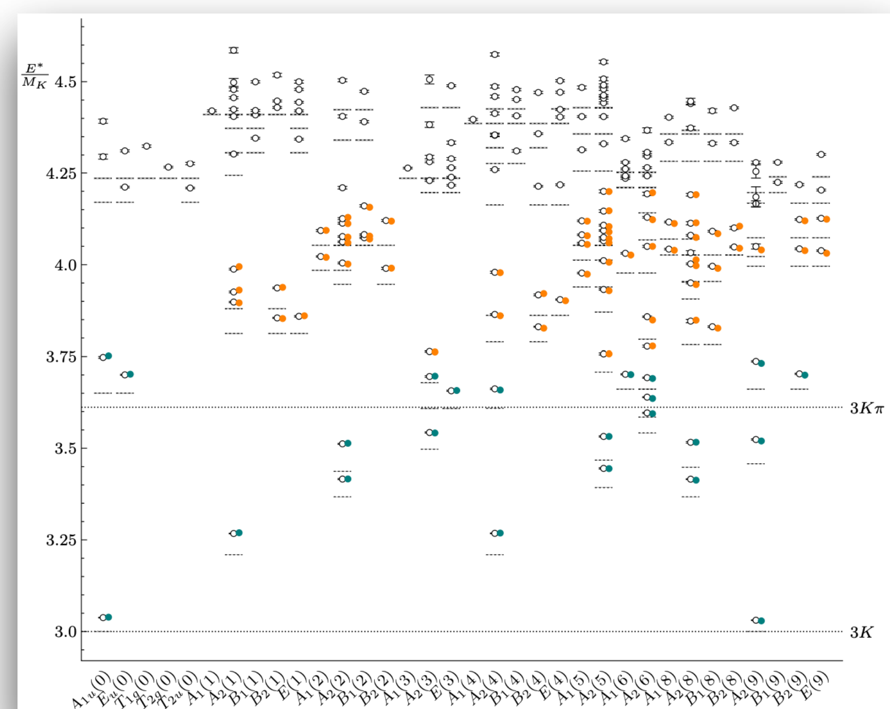
★ Novel developments in relation to the Luscher (and others) formalism for unstable states (transition form factors)

★ At the forefront: reactions involving three-hadron scattering amplitudes accessed via lattice QCD

★ Direction actively pursued: e.g., [Mai et al., PRL 122, 062503 (2019)], [Blanton et al., PRL 124, 032001 (2020)], [Blanton et al., JHEP 10 023 (2021)], [Mai et al., PRD 101, 054510 (2020)] [Guo et al., PRD 101, 094510 (2020)], [Blanton et al., JHEP 10 023 (2021)], [Hansen et al., PRL 126, 012001 (2021)]

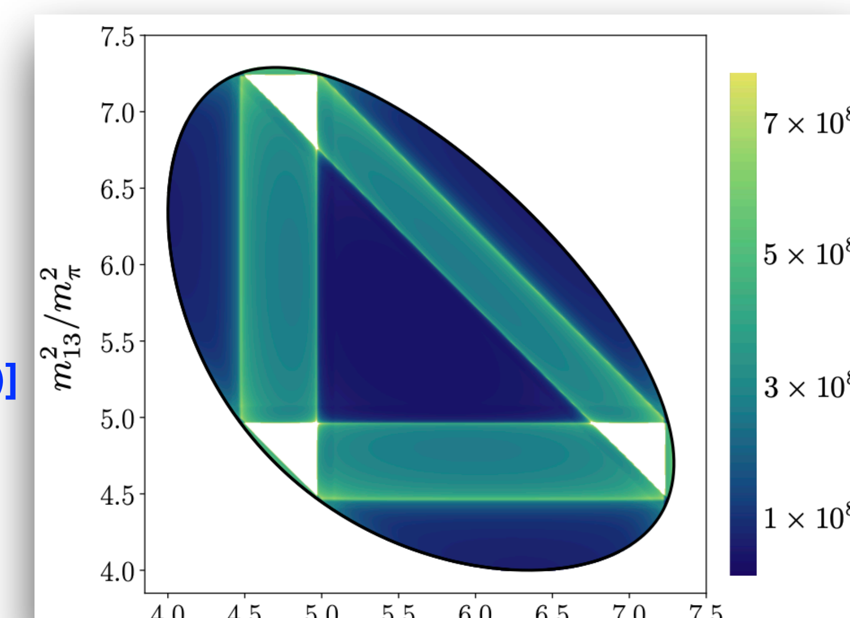
$K^+K^+K^+$ scattering amplitude

[Blanton et al., JHEP 10 023 (2021)]

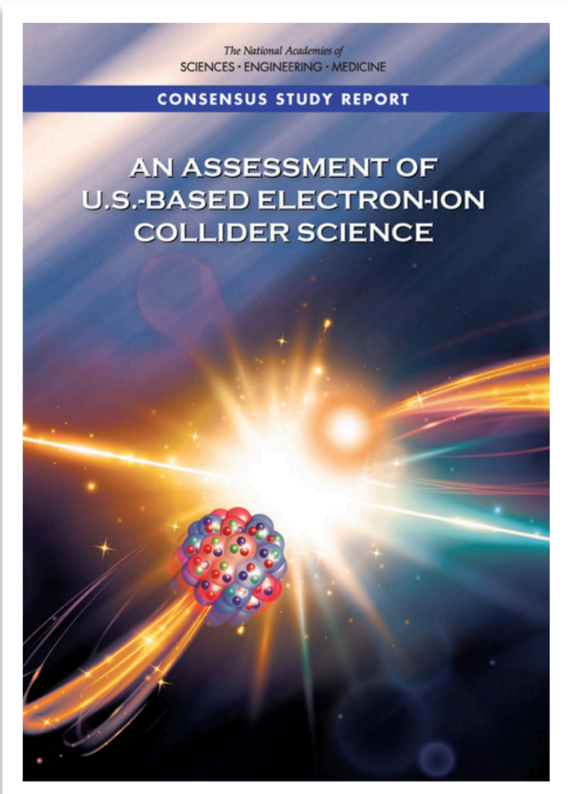


$\pi^+\pi^+\pi^+$ scattering amplitude

[Hansen et al., PRL 126, 012001 (2021)]



Hadron Structure



Main Pillars of NAS Assessment report for EIC

Finding 1: An EIC can uniquely address three profound questions about nucleons—neutrons and protons—and how they are assembled to form the nuclei of atoms:

- How does the mass of the nucleon arise?
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- What are the emergent properties of dense systems of gluons?

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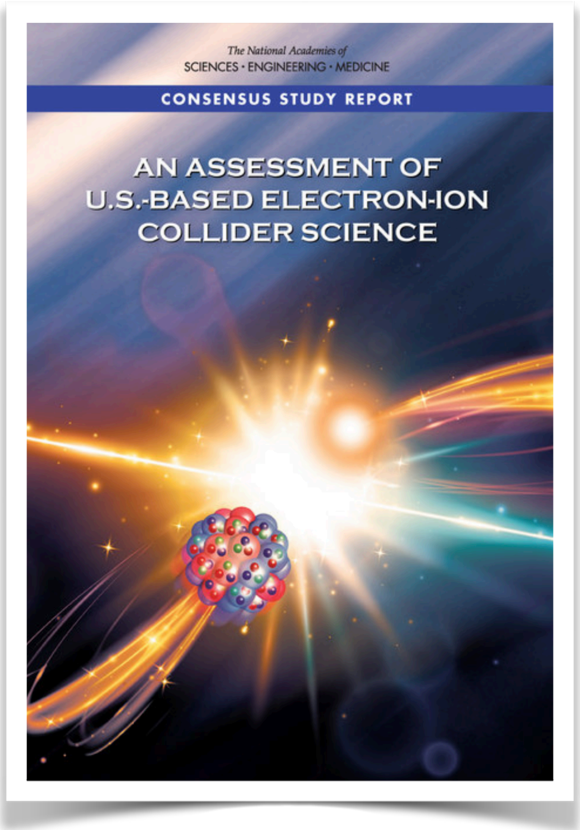

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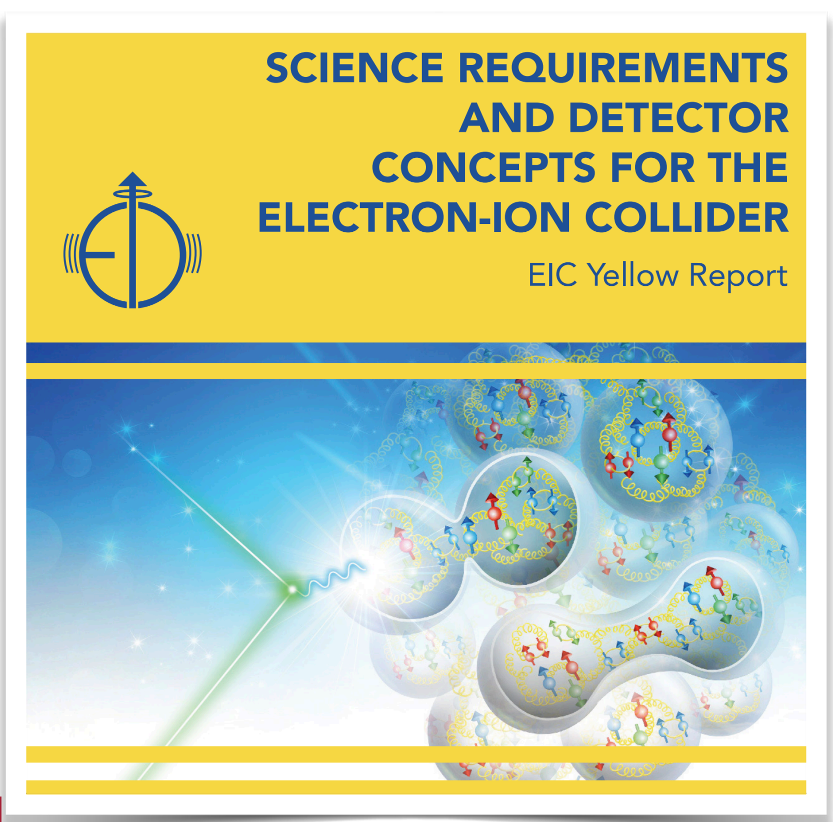

Advances of Lattice QCD are timely

Lattice QCD is featured in the EIC Yellow Report

Lattice QCD can provide valuable input in understanding the proton mass and spin decomposition from *first principles*

Hadron Structure

Proton spin:

★ Significant progress in experiments and global analysis, e.g.

- ⇨ RHIC results on flavor decomposition of antiquarks in spin [J. Adam et al., PRD 99, 051102 (2019)]
- ⇨ First data-driven evidence of nonzero antiquark asymmetry [C. Cocuzza et al., PRD 106, L031502 (2022)]

★ Complete spin decomposition still challenging

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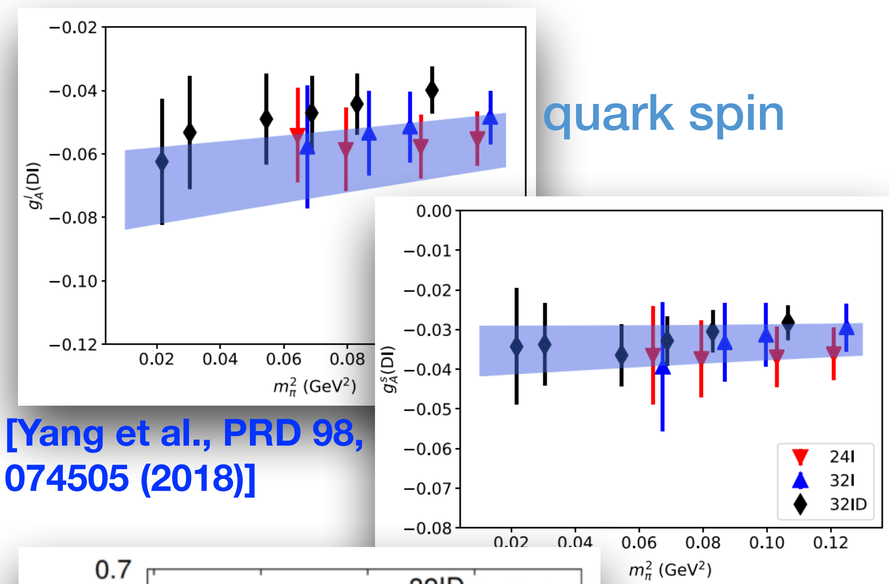
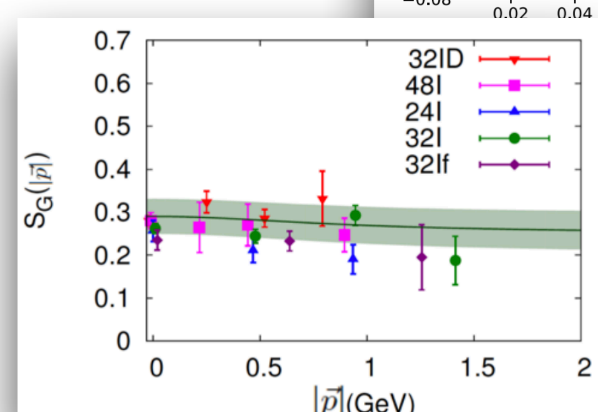


quark spin

[Yang et al., PRD 98, 074505 (2018)]



glue spin

[Yang et al., PRL 118, 102001 (2017)]

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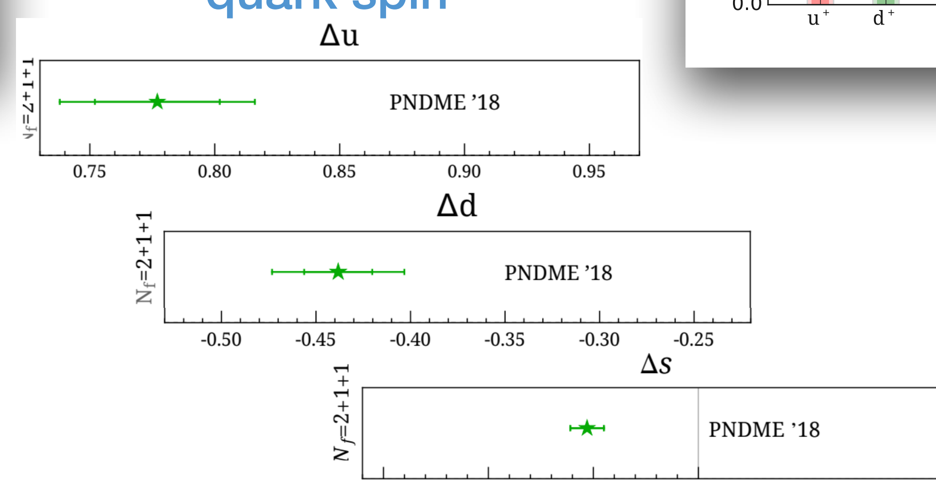

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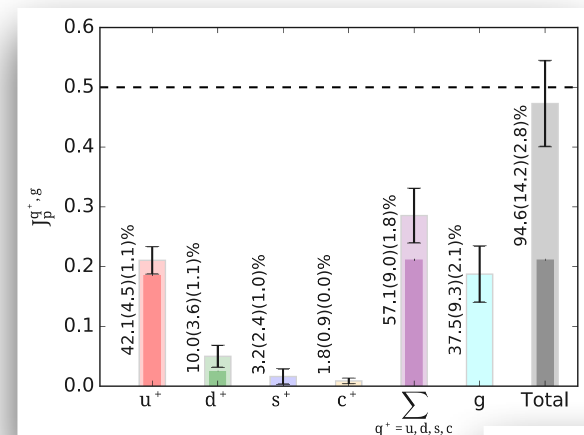

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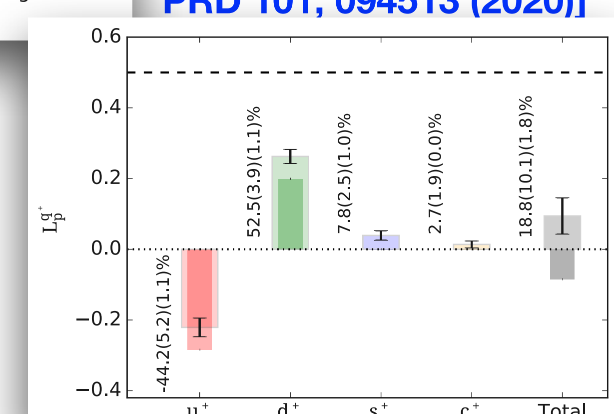

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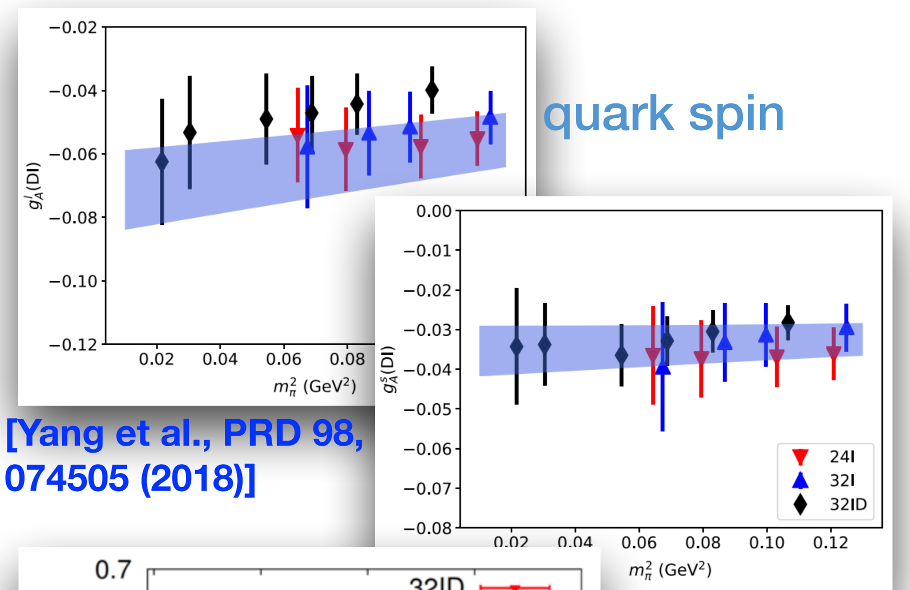

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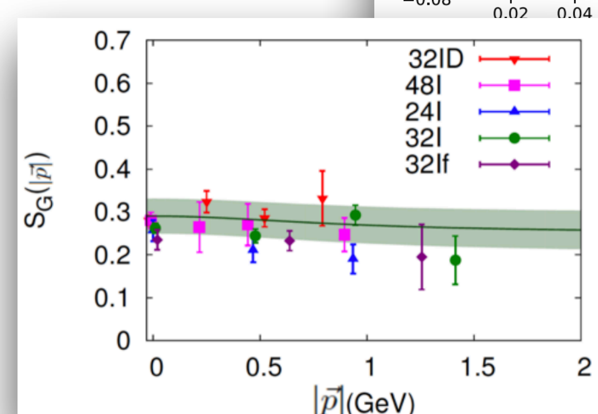

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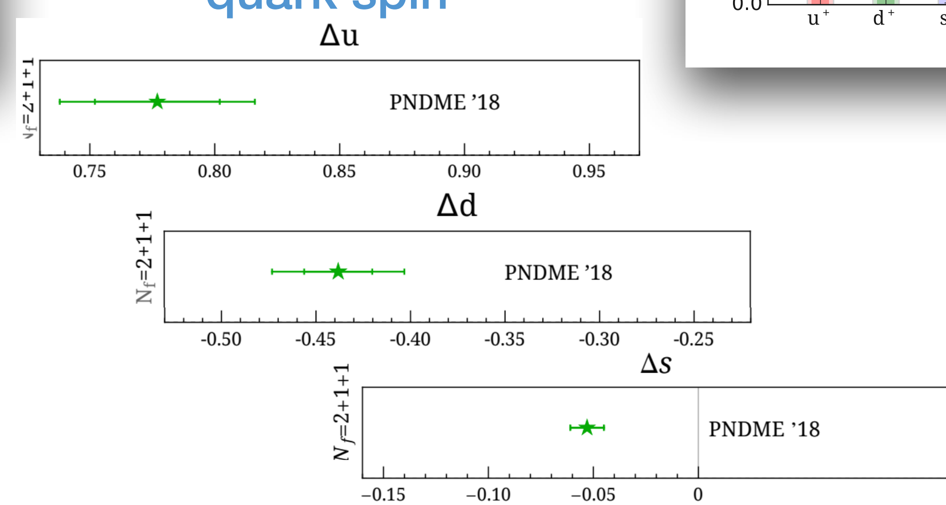

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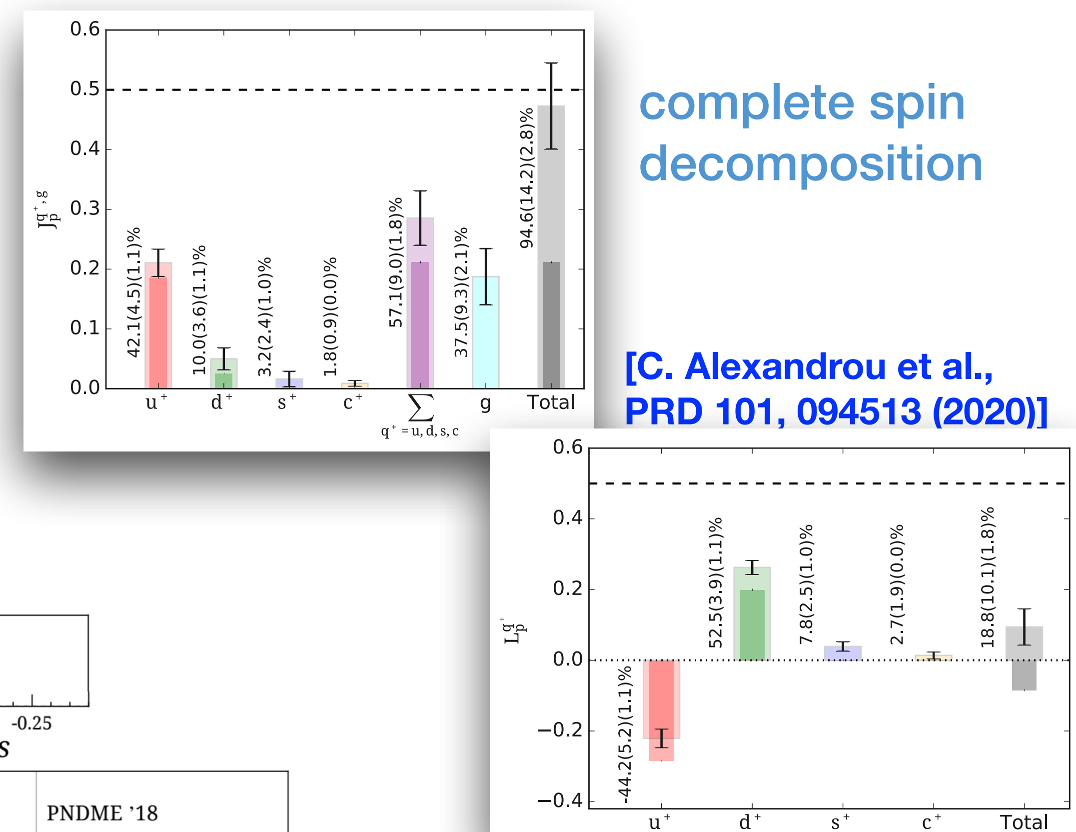

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[C. Alexandrou et al., PRD 101, 094513 (2020)]

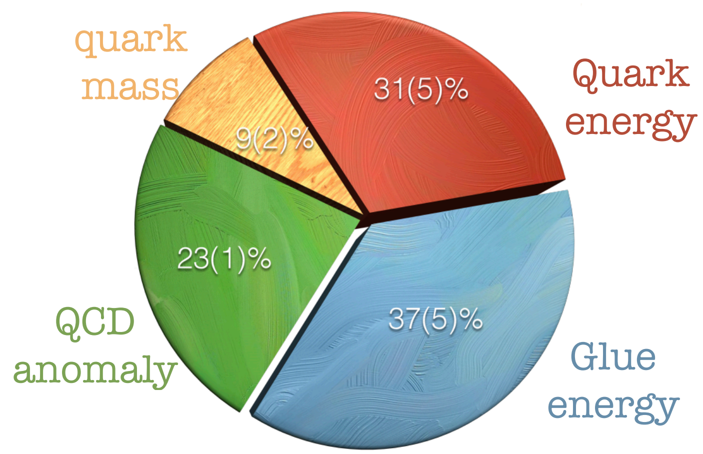
Impressive progress in the field leading to new opportunities

Hadron Structure

Gluon structure

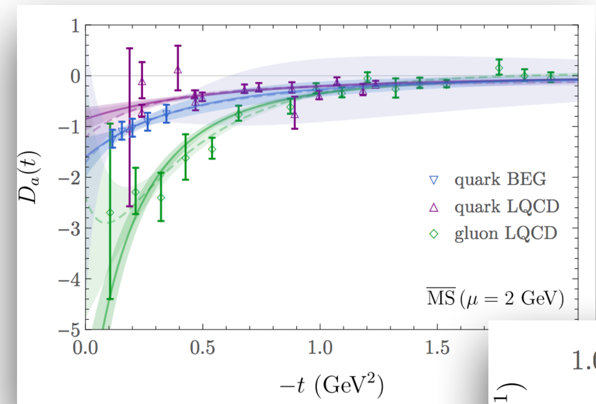
- ★ Dedicated resources and novel methods lead to state-of-the-art results
- ★ Gluon gravitational FFs, pressure distribution & shear forces inside hadron

Proton mass decomposition



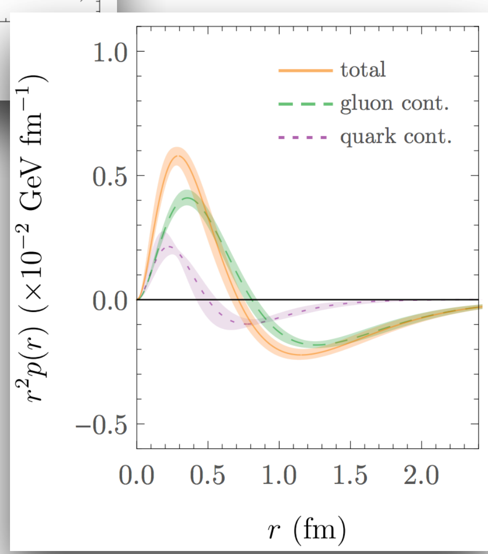
[Yang et al., PRL 121, 212001 (2018)]

gluon gravitational FFs (proton)



[Shanahan et al., PRD 99, 014511 (2019)]

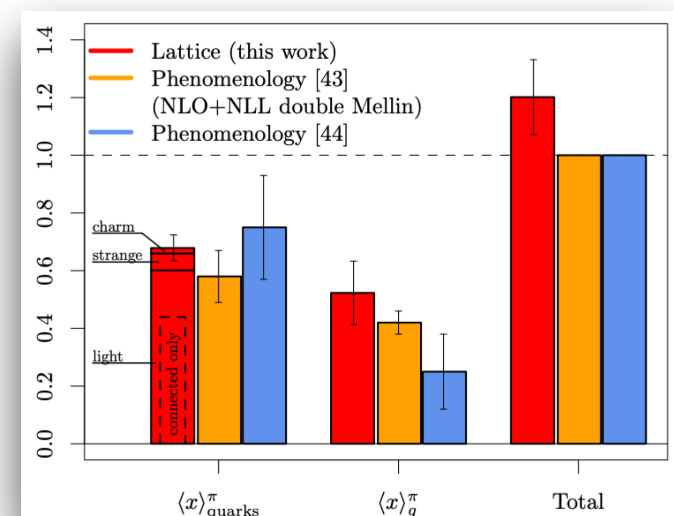
pressure distribution (proton)



[Shanahan et al., PRL 122, 072003 (2019)]

and many more!

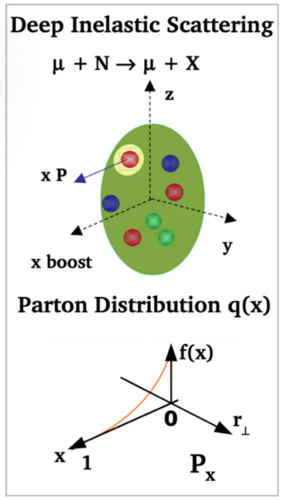
Momentum decomposition in pion



[C. Alexandrou et al., PRL 127, 252001 (2021)]

Hadron Structure

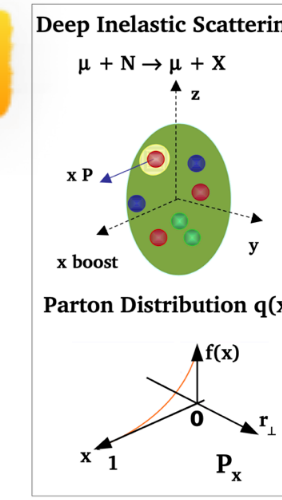
Y. Zhao, Sat 9:30 am



★ Novel program of calculations of x-dependent PDFs of hadrons

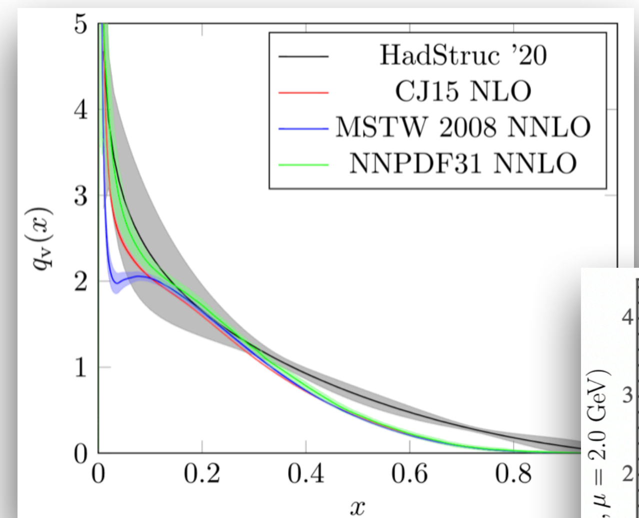
Hadron Structure

Y. Zhao, Sat 9:30 am



★ Novel program of calculations of x-dependent PDFs of hadrons

proton unpolarized quark PDF

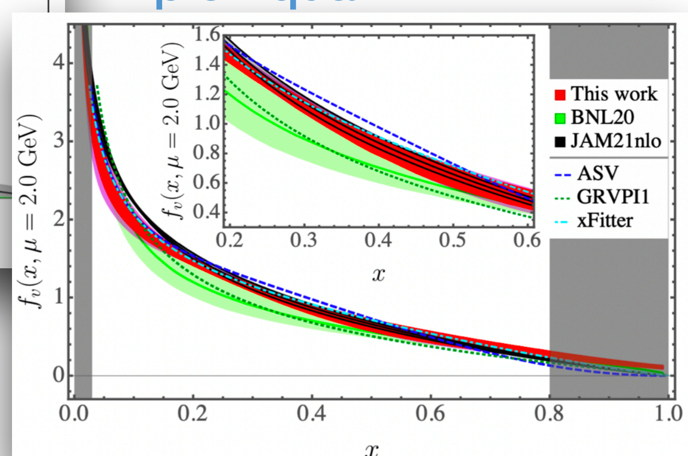


[ETMC (Alexandrou et al.), PRL 121, 112001 (2018)]

[HadStruc (Joo et al.), PRL 125, 23 (2020)]

[ETMC (Bhat et al.), PRD 103, 034510 (2021)]

pion quark PDF



[Yong Zhao et al., PRL 128, 142003 (2022)]

Hadron Structure

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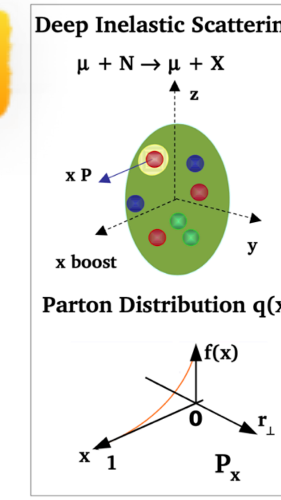

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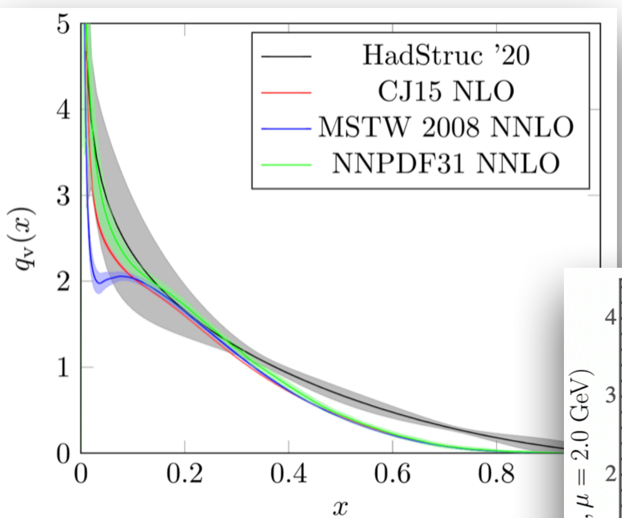

[ETMC (Alexandrou et al.), PRL 121, 112001 (2018)]
[HadStruc (Joo et al.), PRL 125, 23 (2020)]
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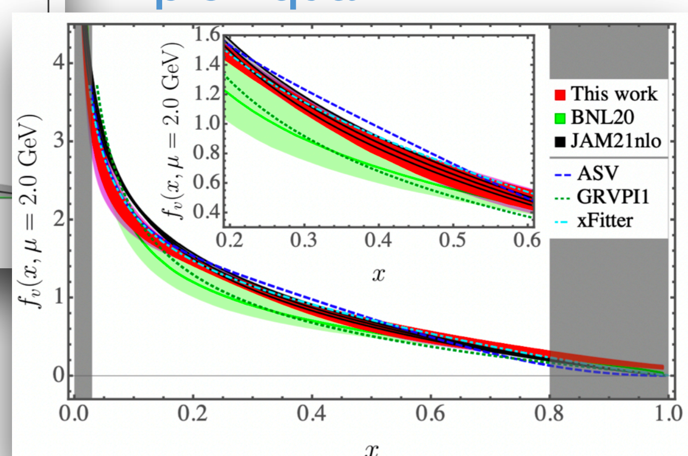
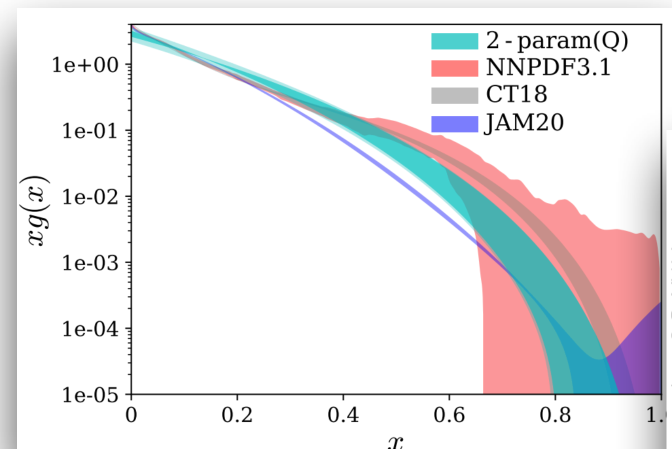
pion quark PDF



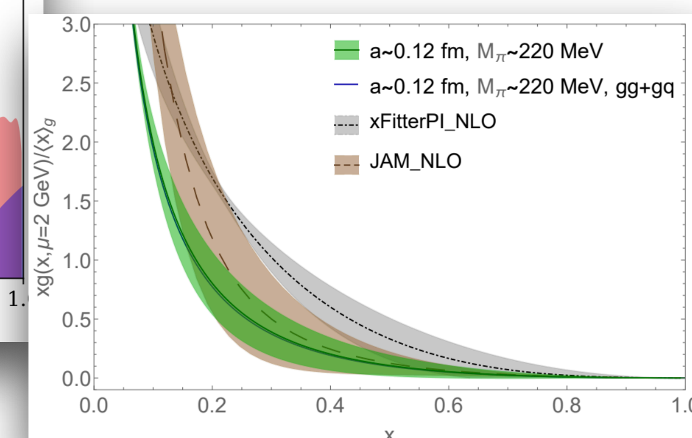
[Yong Zhao et al., PRL 128, 142003 (2022)]

proton unpolarized gluon PDF



[HadStruc (Khan et al.) JHEP 11, 148 (2021)]

pion gluon PDF

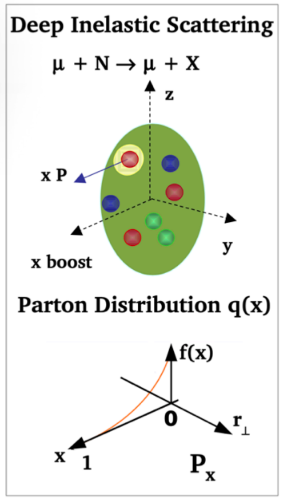


[Fan et al., PLB 823, 136778 (2021)]

Statistical uncertainties of lattice calculations under control

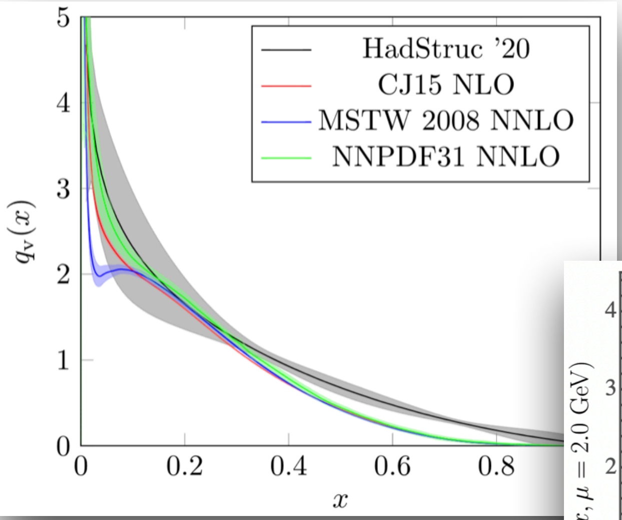
Hadron Structure

Y. Zhao, Sat 9:30 am



★ Novel program of calculations of x-dependent PDFs of hadrons

proton unpolarized quark PDF



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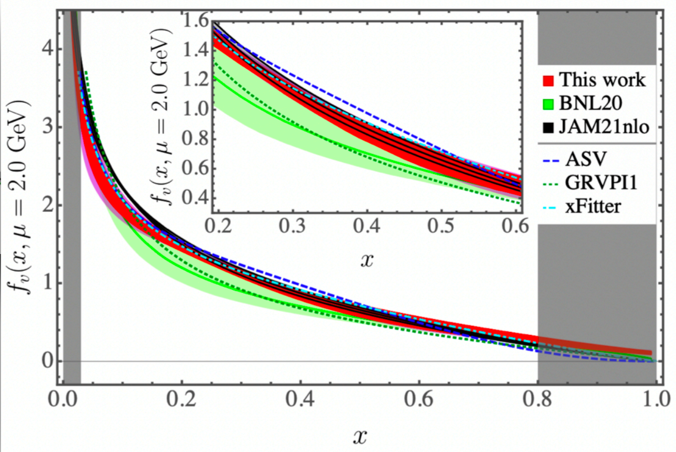
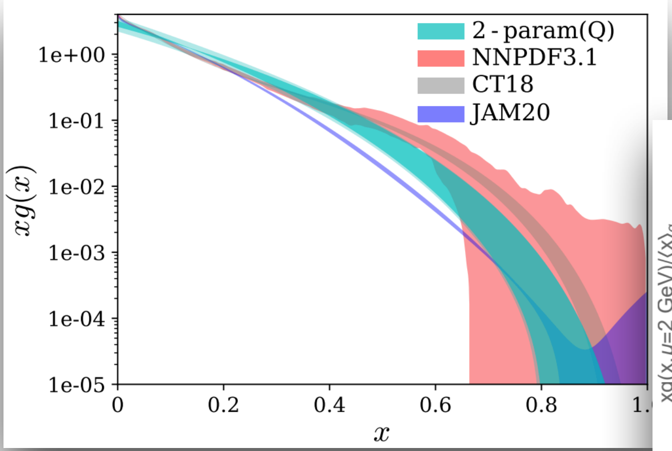
[ETMC (Bhat et al.), PRD 103, 034510 (2021)]

pion quark PDF



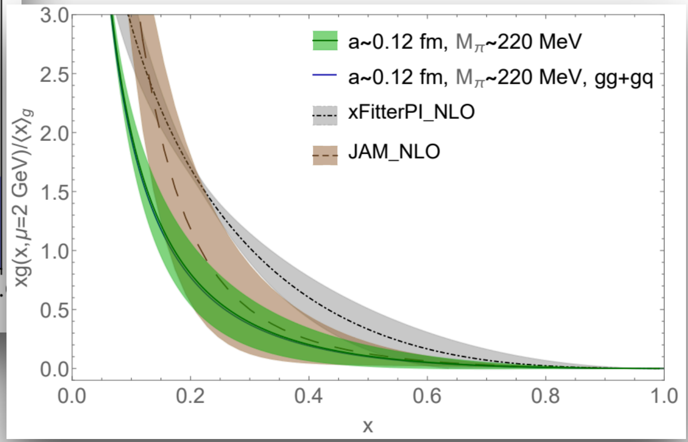
[Yong Zhao et al., PRL 128, 142003 (2022)]

proton unpolarized gluon PDF



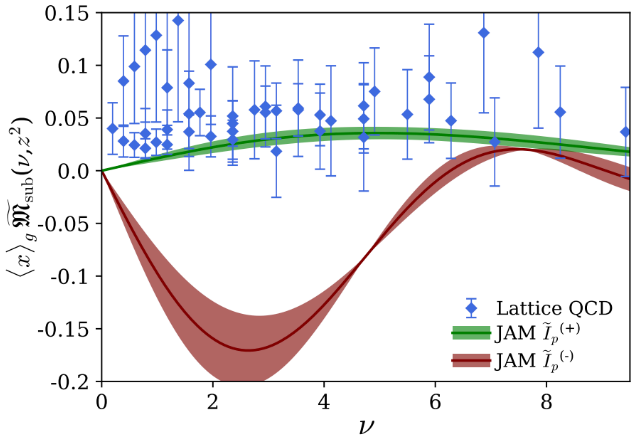
[HadStruc (Khan et al.) JHEP 11, 148 (2021)]

pion gluon PDF



[Fan et al., PLB 823, 136778 (2021)]

proton gluon helicity PDF



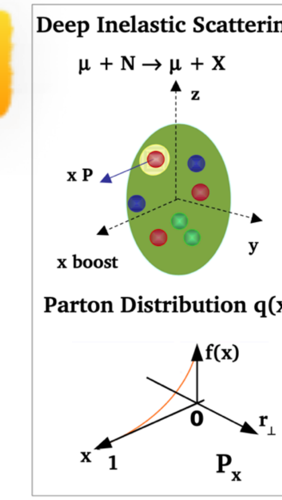
[HadStruc (Egerer et al.) arXiv:2207.08733]

Statistical uncertainties of lattice calculations under control

Comparison of Ioffe-time gluon helicity PDF with JAM analysis: new findings on assumption of positivity constraints

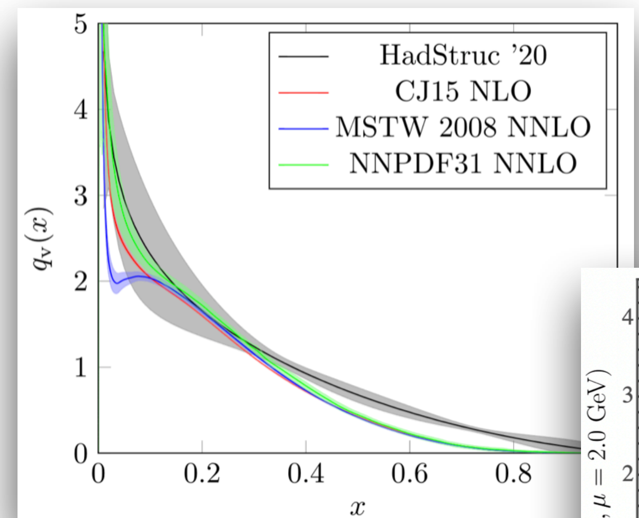
Hadron Structure

Y. Zhao, Sat 9:30 am



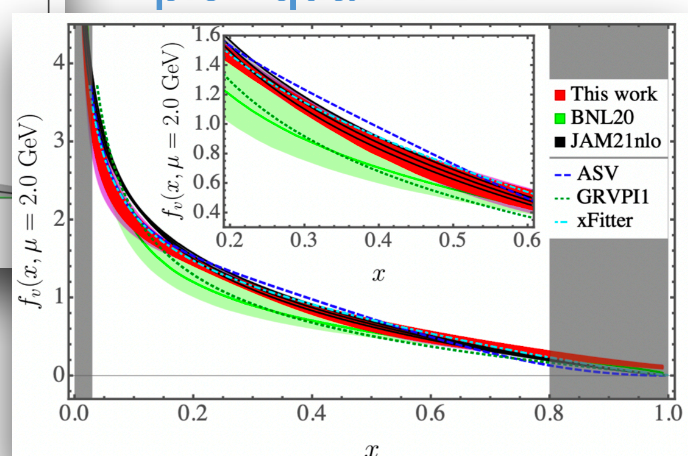
★ Novel program of calculations of x-dependent PDFs of hadrons

proton unpolarized quark PDF



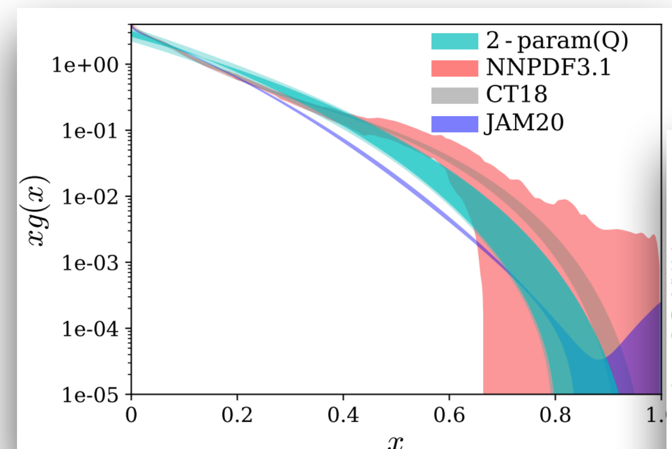
[ETMC (Alexandrou et al.), PRL 121, 112001 (2018)]
[HadStruc (Joo et al.), PRL 125, 23 (2020)]
[ETMC (Bhat et al.), PRD 103, 034510 (2021)]

pion quark PDF



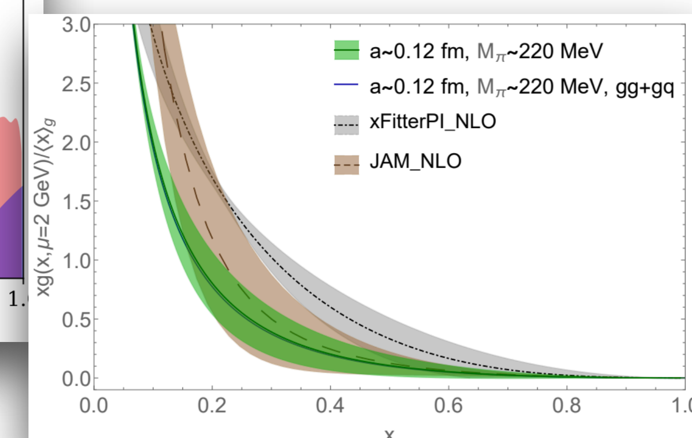
[Yong Zhao et al., PRL 128, 142003 (2022)]

proton unpolarized gluon PDF



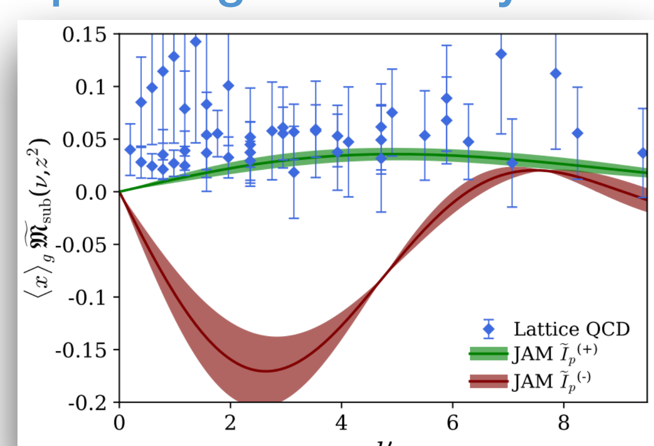
[HadStruc (Khan et al.) JHEP 11, 148 (2021)]

pion gluon PDF



[Fan et al., PLB 823, 136778 (2021)]

proton gluon helicity PDF



[HadStruc (Egerer et al.) arXiv:2207.08733]

Statistical uncertainties of lattice calculations under control

Comparison of Ioffe-time gluon helicity PDF with JAM analysis: new findings on assumption of positivity constraints

Lattice QCD can provide key information in the pre-EIC era

Nuclear Forces and Nuclei

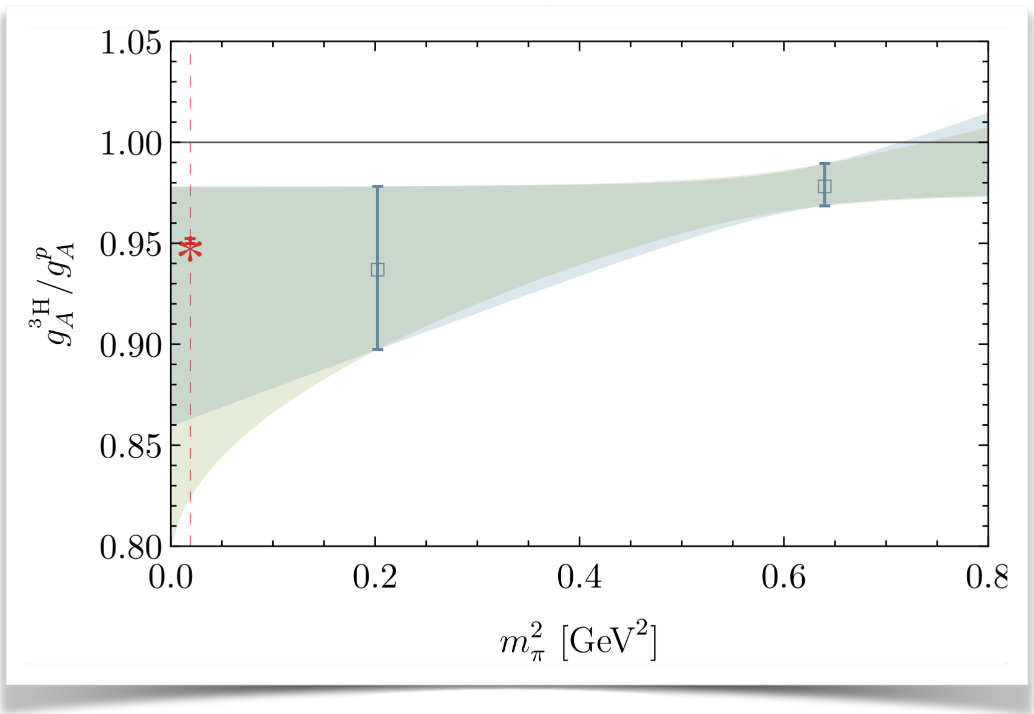
★ Lattice QCD calculations address multi-baryon interactions

⇨ understand connection between QCD and nuclear physics

⇨ complement nuclear models and EFTs:

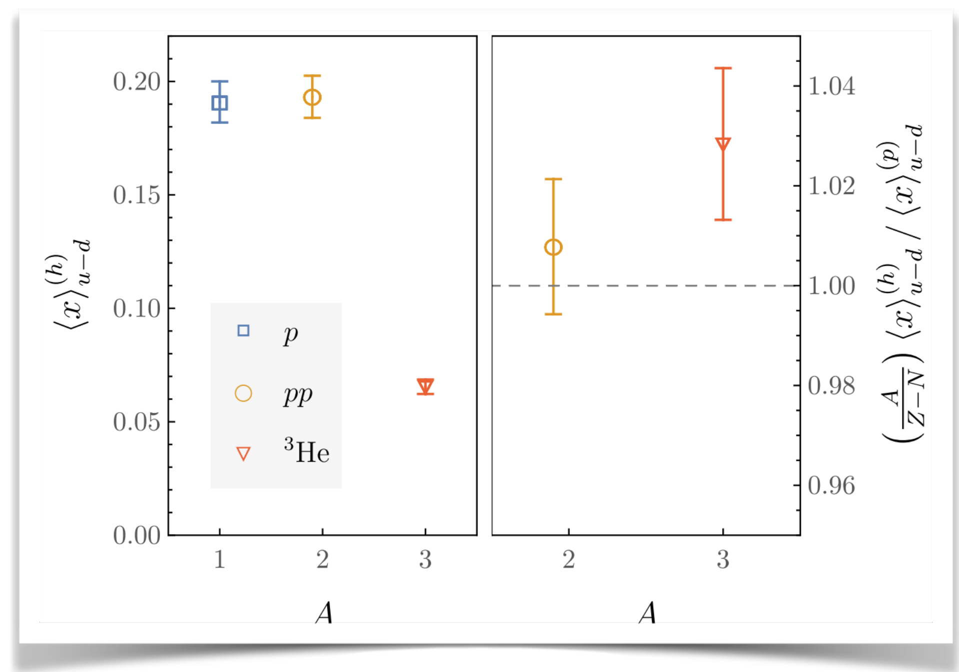
double-beta decay, neutrino-nucleus scattering, electroweak reaction rates, …

axial charge of triton



[NPLQCD (Parreño et al.) , PRD 103 (2021) 074511]

Longitudinal momentum fraction

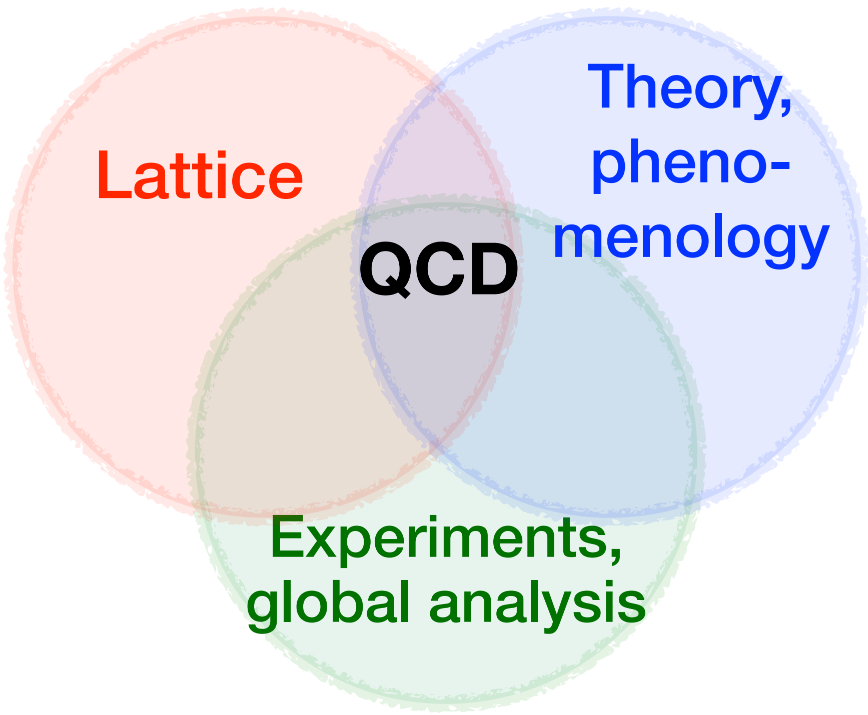


[NPLQCD (Detmold et al.), PRL 126 (2021) 202001]

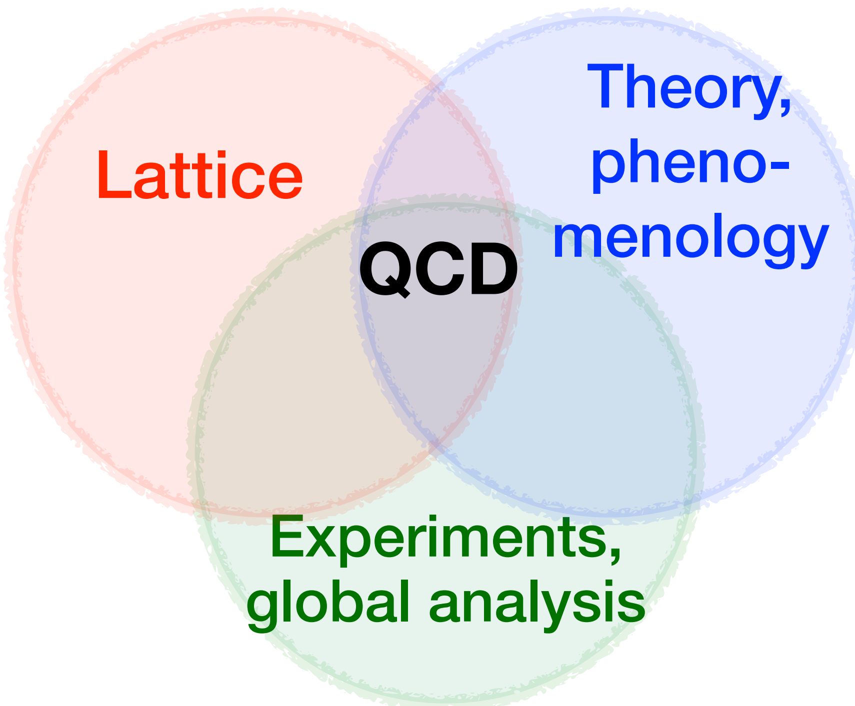
★ Limited proof-of-concept calculations, but show promising qualitative results

★ Exascale computing era will advance studies of multi-baryon interactions

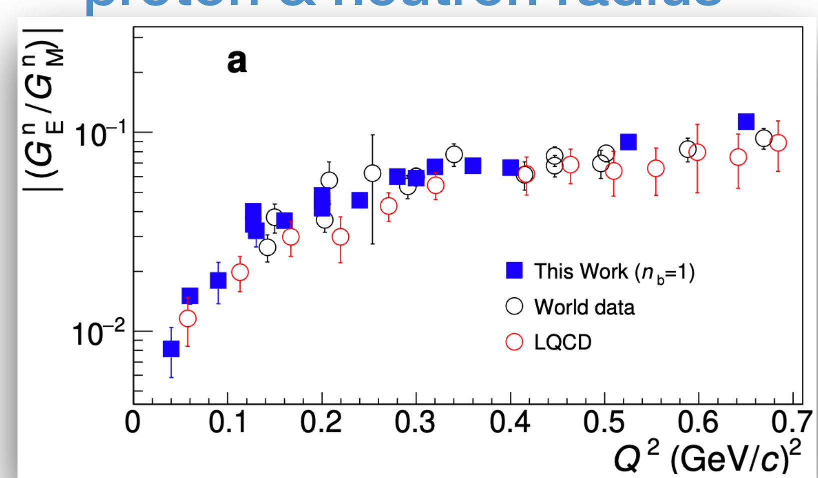
Synergies: constraints & predictive power of lattice QCD



Synergies: constraints & predictive power of lattice QCD

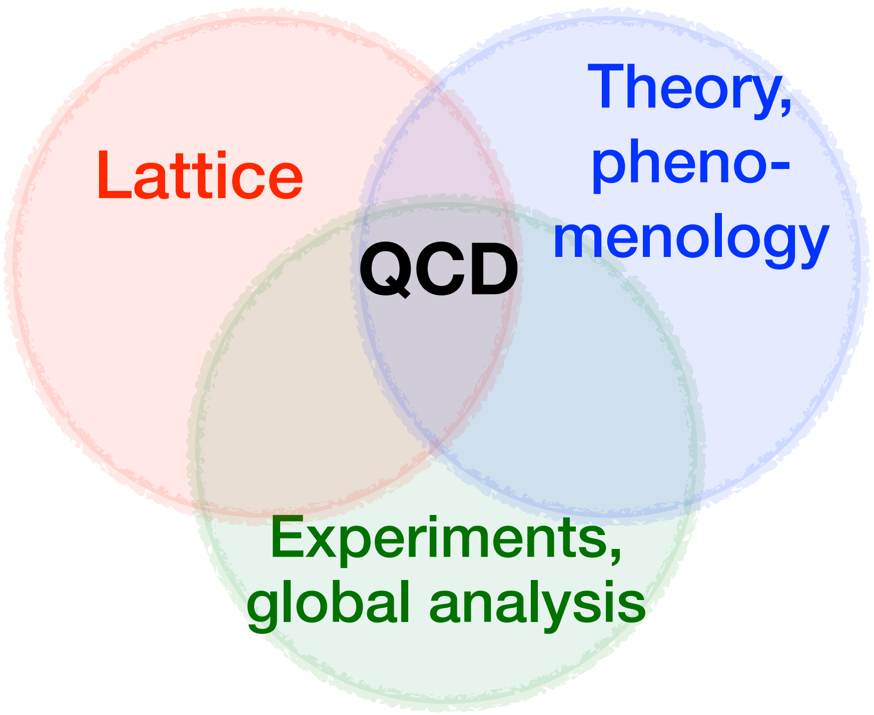


proton & neutron radius

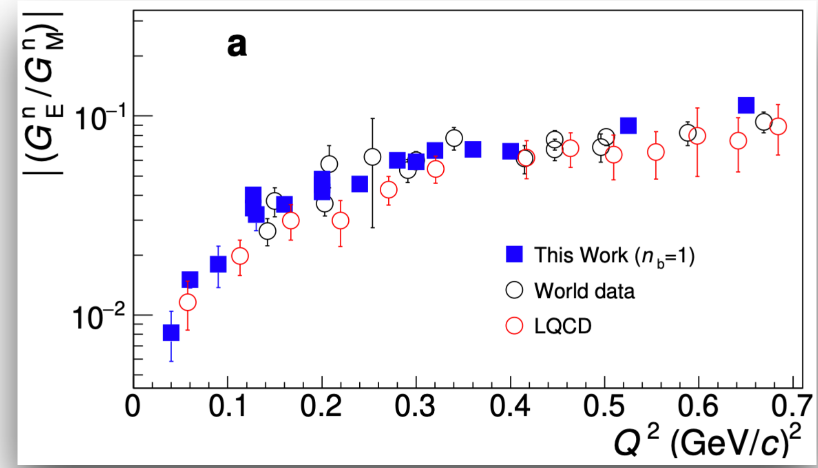


[Atac et al., Nature Comm. 12, 1759 (2021)]

Synergies: constraints & predictive power of lattice QCD

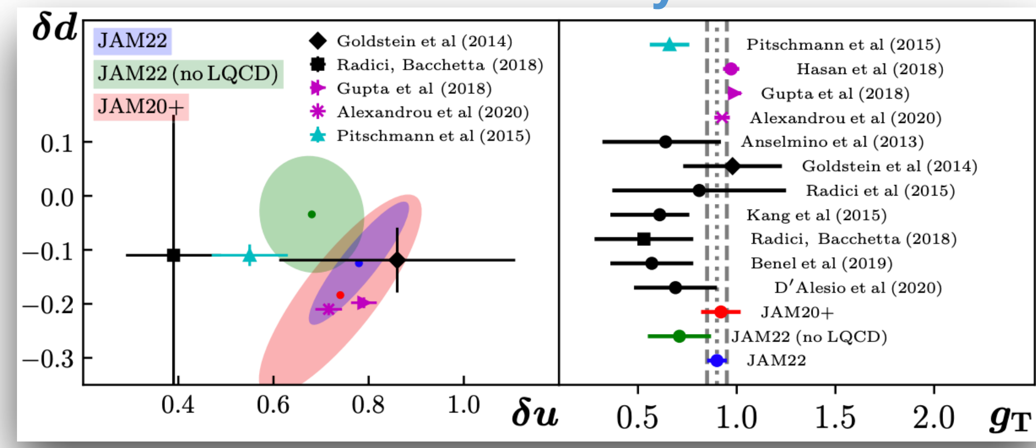


proton & neutron radius



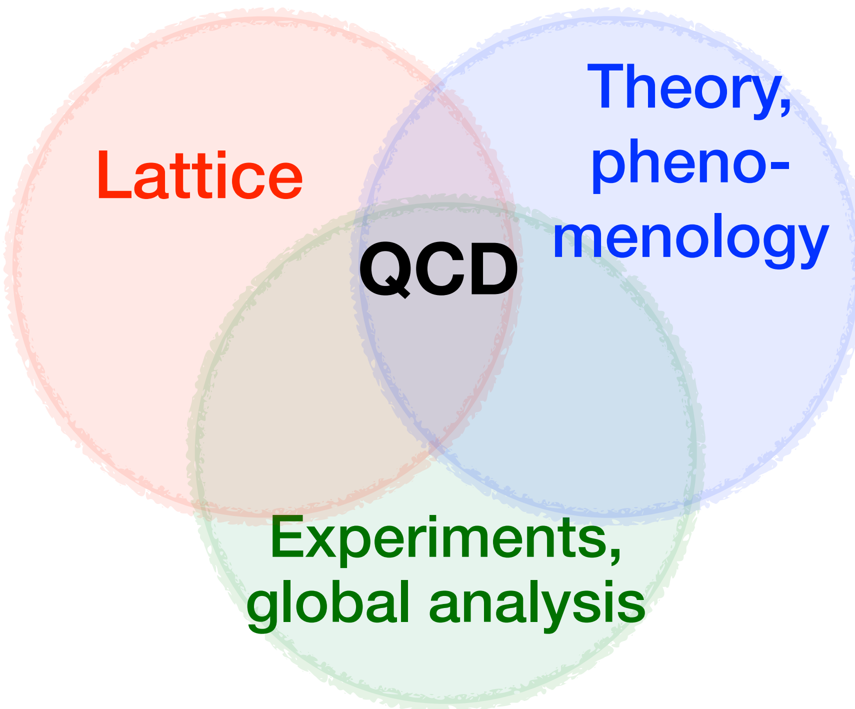
[Atac et al., Nature Comm. 12, 1759 (2021)]

transversity PDF



[JAM, PRD 106 (2022) 3, 034014]

Synergies: constraints & predictive power of lattice QCD



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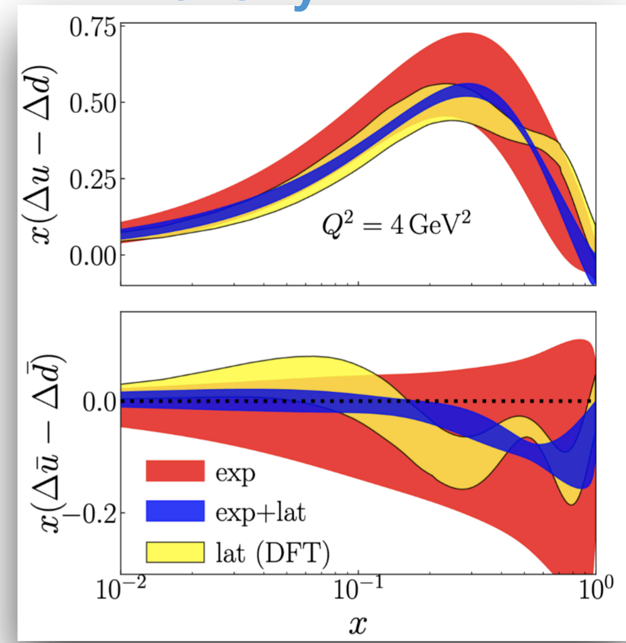
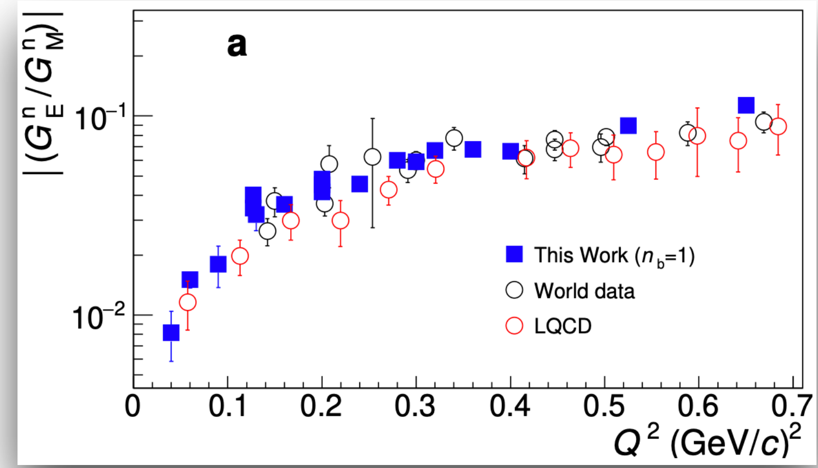


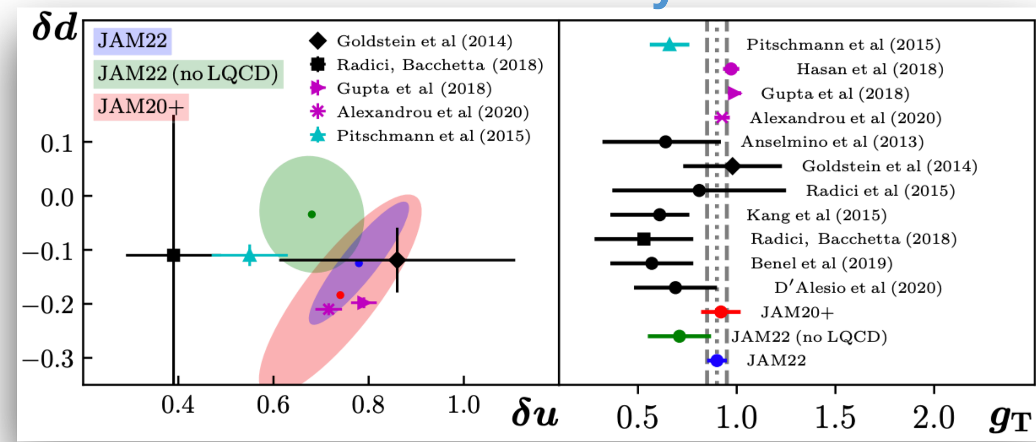
[JAM & ETMC, PRD 103 (2021) 016003]

proton & neutron radius



[Atac et al., Nature Comm. 12, 1759 (2021)]

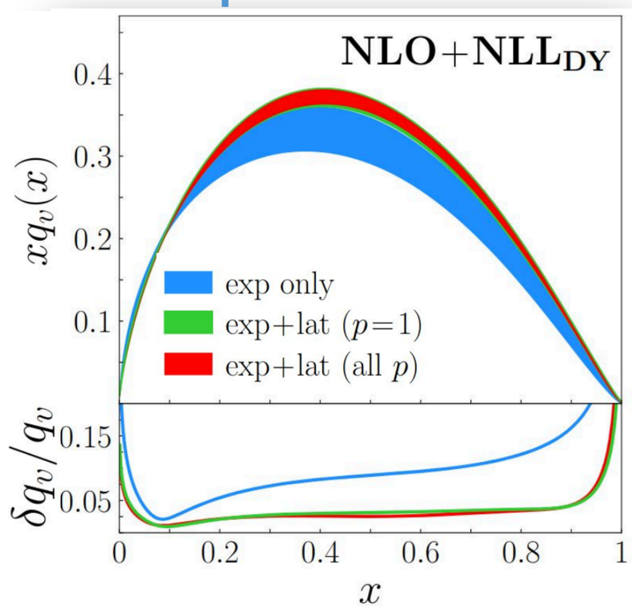
transversity PDF



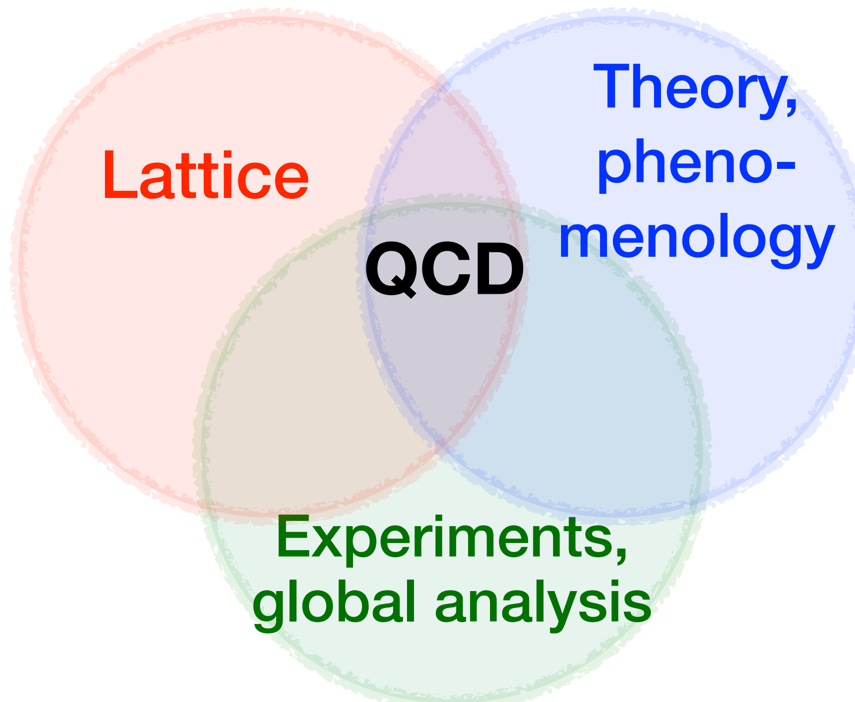
[JAM, PRD 106 (2022) 3, 034014]

Synergies: constraints & predictive power of lattice QCD

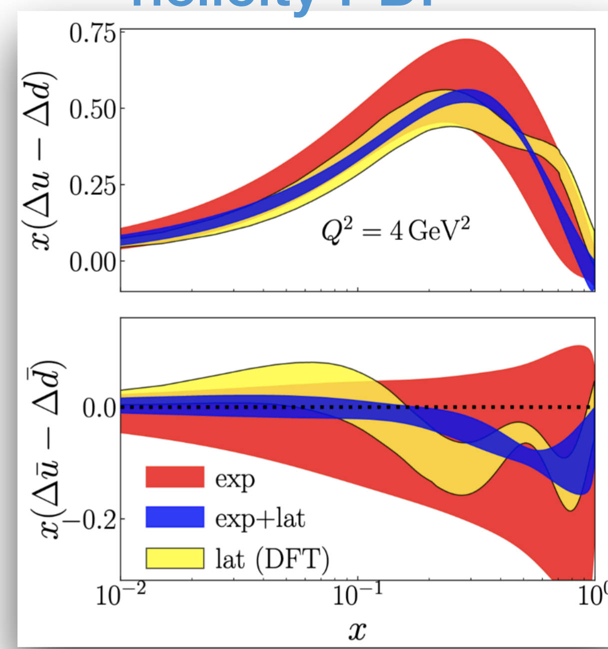
pion PDF



[JAM/HadStruc, PRD105 (2022) 114051]

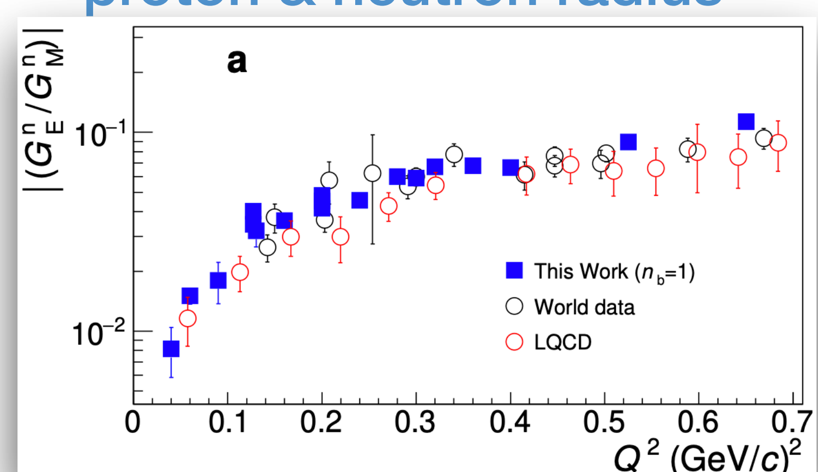


helicity PDF



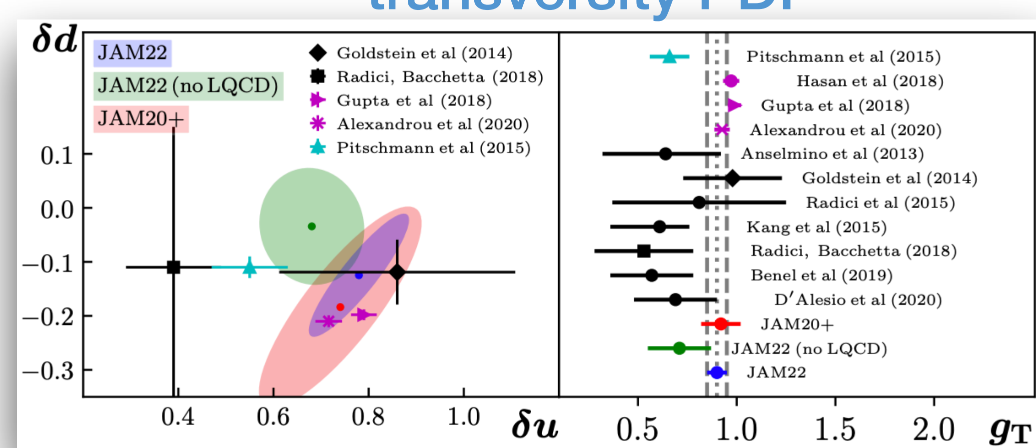
[JAM & ETMC, PRD 103 (2021) 016003]

proton & neutron radius



[Atac et al., Nature Comm. 12, 1759 (2021)]

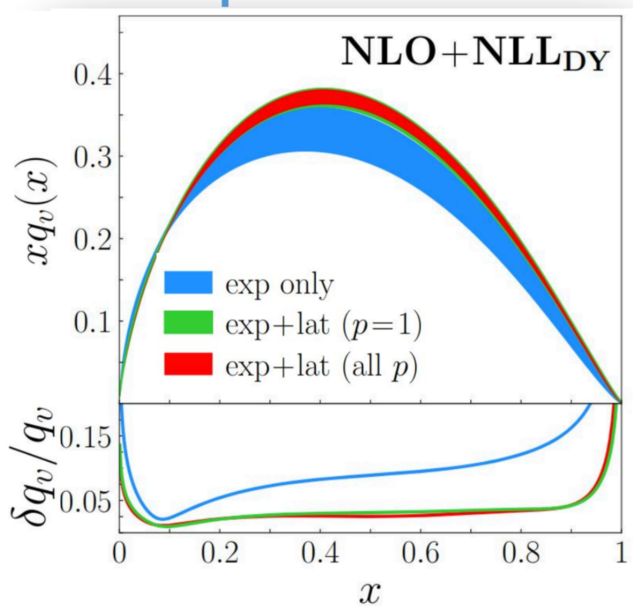
transversity PDF



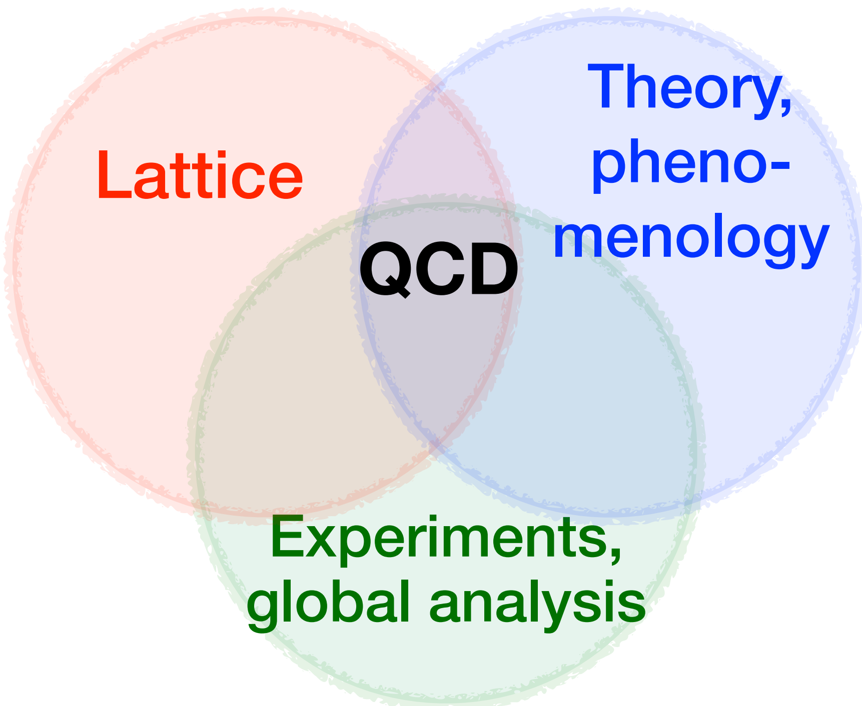
[JAM, PRD 106 (2022) 3, 034014]

Synergies: constraints & predictive power of lattice QCD

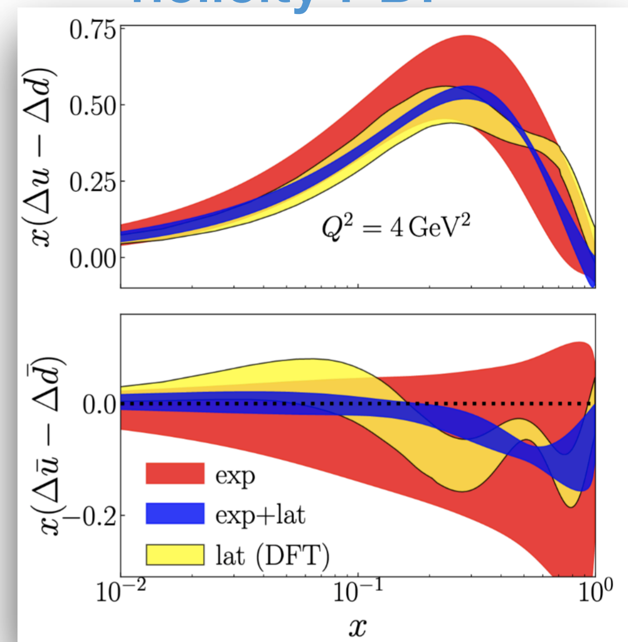
pion PDF



[JAM/HadStruc, PRD105 (2022) 114051]

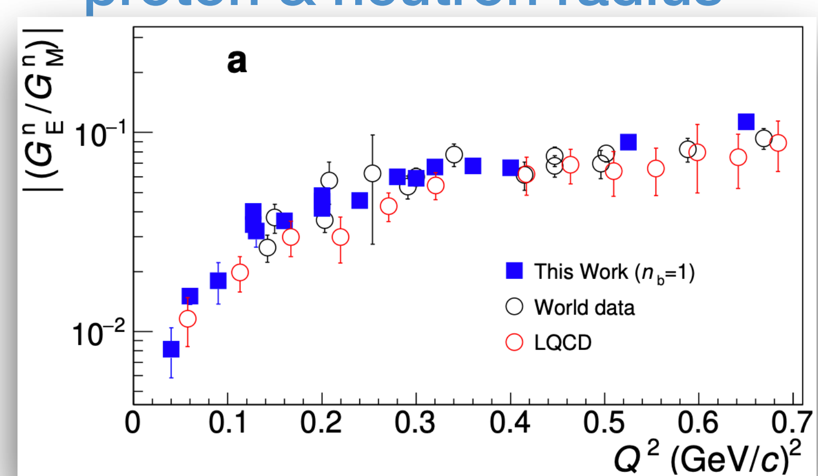


helicity PDF



[JAM & ETMC, PRD 103 (2021) 016003]

proton & neutron radius



[Atac et al., Nature Comm. 12, 1759 (2021)]

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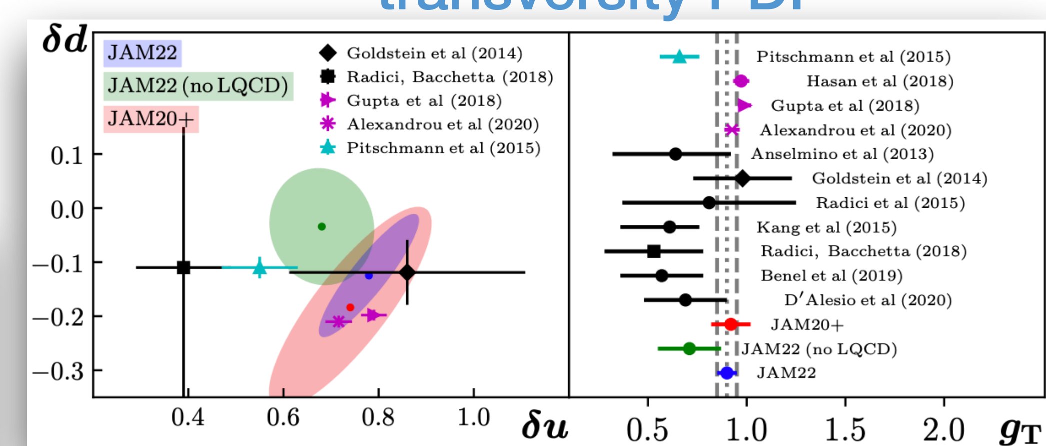
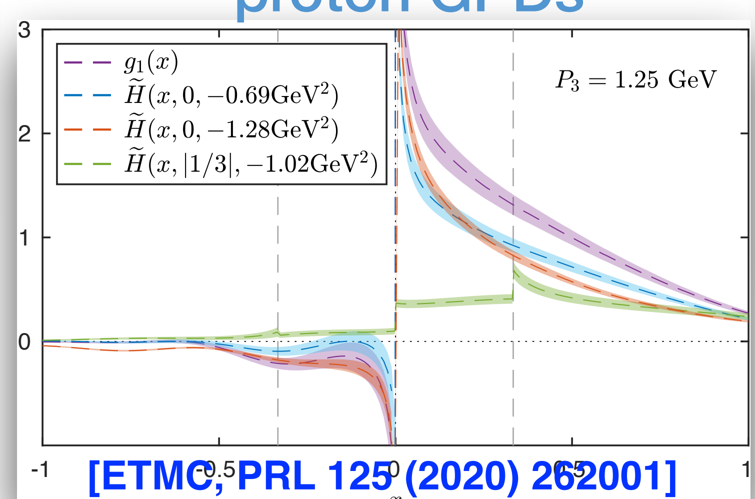


[JAM, PRD 106 (2022) 3, 034014]

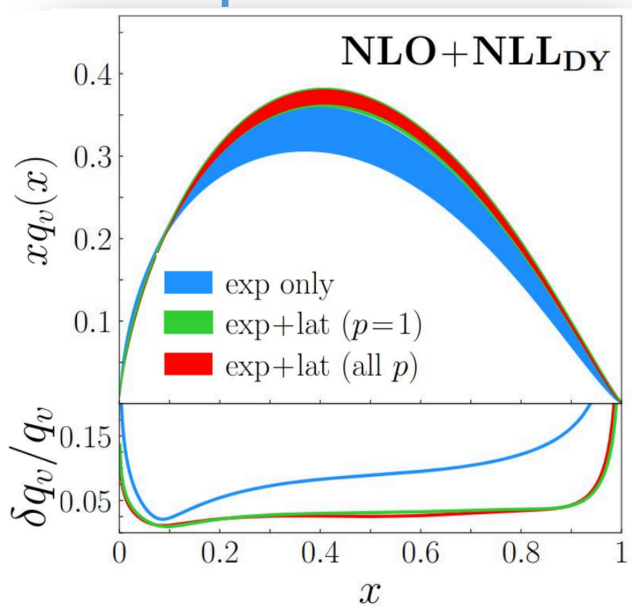
proton GPDs



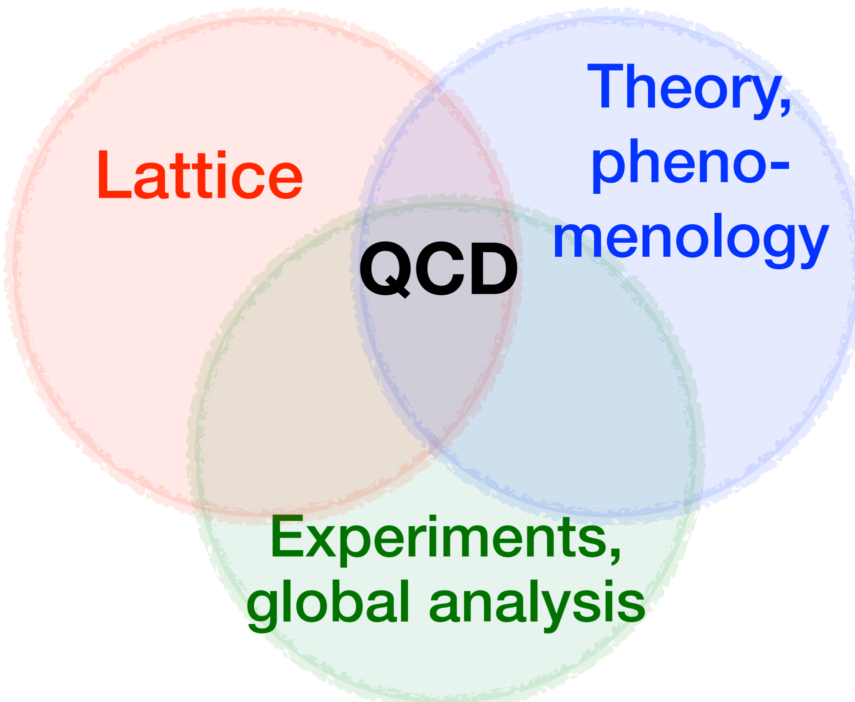
[ETMC, PRL 125 (2020) 262001]

Synergies: constraints & predictive power of lattice QCD

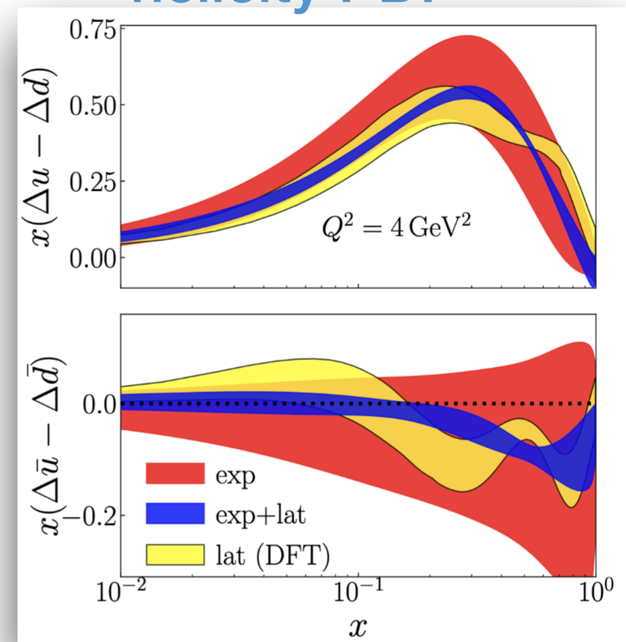
pion PDF



[JAM/HadStruc, PRD105 (2022) 114051]

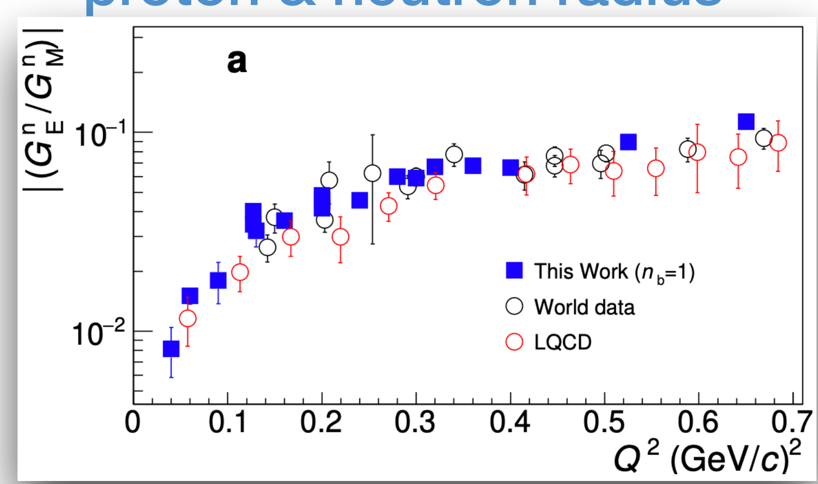


helicity PDF



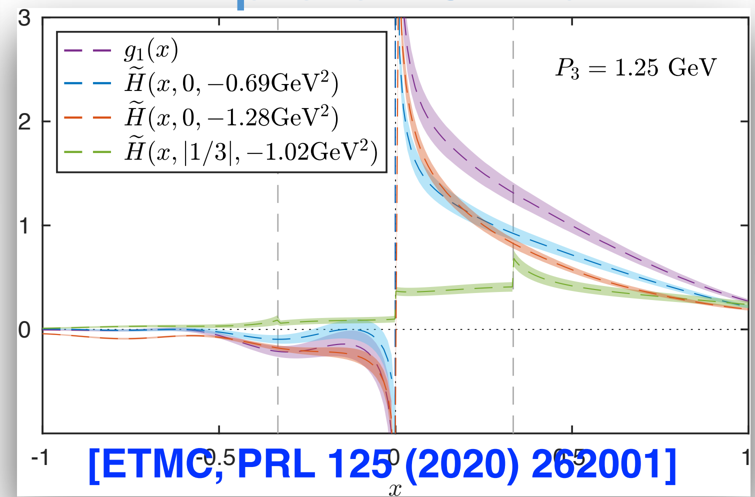
[JAM & ETMC, PRD 103 (2021) 016003]

proton & neutron radius



[Atac et al., Nature Comm. 12, 1759 (2021)]

proton GPDs



[ETMC, PRL 125 (2020) 262001]

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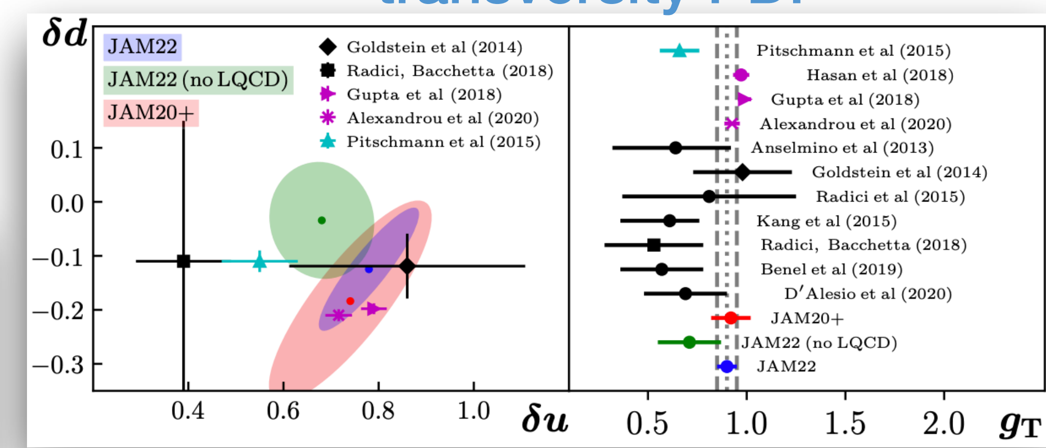

[JAM, PRD 106 (2022) 3, 034014]

And many more!

USQCD and 2020-2022 Snowmass

APS | DIVISION OF PARTICLES & FIELDS

★ Strong USQCD presence in frontiers (conveners and topical group leaders):

- ⇨ Computational Frontier: Theoretical Calculations & Simulations; Machine Learning, Quantum Computing
- ⇨ Theory Frontier: Lattice Gauge Theory; QIS
- ⇨ Energy Frontier: QCD hadron structure, QCD heavy ions
- ⇨ Rare Processes and Precision: Weak Decays of b and c Quarks; Fundamental Physics in Small Experiments; Hadronic Spectroscopy

★ Several LOI and whitepapers

Lattice QCD and the Computational Frontier

Peter Boyle[a,b], Dennis Bollweg[c], Richard Brower[d], Norman Christ[c], Carleton DeTar[e], Robert Edwards[f], Steven Gottlieb[g], Taku Izubuchi[a,h], Balint Joo[i], Fabian Joswig[b], Chulwoo Jung[a], Christopher Kelly[k], Andreas Kronfeld[j], Meifeng Lin[k], James Osborn[l], Antonin Portelli[b], James Richings[b], Azusa Yamaguchi[b]

A lattice QCD perspective on weak decays of b and c quarks
Snowmass 2022 White Paper

Peter A. Boyle,[1,2] Bipasha Chakraborty,[3] Christine T. H. Davies,[4] Thomas DeGrand,[5] Carleton DeTar,[6] Luigi Del Debbio,[2] Aida X. El-Khadra,[7] Felix Erben,[2] Jonathan M. Flynn,[8] Elvira Gámiz,[9] Davide Giusti,[10] Steven Gottlieb,[11] Maxwell T. Hansen,[2] Jochen Heitger,[12] Ryan Hill,[2] William I. Jay,[13] Andreas Jüttner,[8,14,15] Jonna Koponen,[16] Andreas Kronfeld,[17] Christoph Lehner,[10] Andrew T. Lytle,[7,*] Guido Martinelli,[18] Stefan Meinel,[19] Christopher J. Monahan,[20,21] Ethan T. Neil,[5] Antonin Portelli,[2] James N. Simone,[17] Silvano Simula,[22] Rainer Sommer,[23,24] Amarjit Soni,[1] J. Tobias Tsang,[25] Ruth S. Van de Water,[17] Alejandro Vaquero,[6] Ludovico Vittorio,[26] and Oliver Witzel[27,†]

Lattice QCD Calculations of Parton Physics

Martha Constantinou,[1] Luigi Del Debbio,[2] Xiangdong Ji,[3] Huey-Wen Lin,[4,5] Keh-Fei Liu,[6] Christopher Monahan,[7,8] Kostas Orginos,[7,8] Peter Petreczky,[9] Jian-Wei Qiu,[8] David Richards,[8] Nobuo Sato,[8] Phiala Shanahan,[10] C.-P. Yuan,[4] Jian-Hui Zhang,[11] and Yong Zhao[12]

Discovering new physics in rare kaon decays

Thomas Blum[a], Peter Boyle[b,c], Mattia Bruno[l,k], Norman Christ[e], Felix Erben[c], Xu Feng[g], Vera Guelpers[c], Ryan Hill[c], Raoul Hodgson[c], Danel Hoying[b], Taku Izubuchi[h,b], Yong-Chull Jang[e], Luchang Jin[a], Chulwoo Jung[b], Joe Karpie[e], Christopher Kelly[b], Christoph Lehner[i], Antonin Portelli[c], Christopher Sachrajda[j], Amarjit Soni[g], Masaaki Tomii[a], Bigeng Wang[e,f] and Tianle Wang[e,b]

Applications of Machine Learning to Lattice Quantum Field Theory
Snowmass 2022 White Paper

Denis Boyda,[1,2] Salvatore Calì,[3,2] Sam Foreman,[1] Lena Funcke,[3,2,4] Daniel C. Hackett,[3,2,*] Yin Lin,[3,2] Gert Aarts,[5,6] Andrei Alexandru,[7,8] Xiao-Yong Jin,[1,9] Biagio Lucini,[10,11] and Phiala E. Shanahan[3,2,4]

Hadron Spectroscopy with Lattice QCD*

John Bulava[1], Raúl Briceño[2,3], William Detmold[4,5], Michael Döring[6,2], Robert G. Edwards[2], Anthony Francis[7,8,9], Francesco Knechtli[10], Randy Lewis[11], Sasa Prelovsek[12,13,†], Sinéad M. Ryan[14], Akaki Rusetsky[15,16], Stephen R. Sharpe[17], Adam Szczepaniak[2,18,19], Christopher E. Thomas[20], Michael L. Wagman[21], Marc Wagner[22,23]

Quantum Simulation for High Energy Physics

Christian W. Bauer,[1,a] Zohreh Davoudi,[2,b] A. Baha Balantekin,[3] Tanmoy Bhattacharya,[4] Marcela Carena,[5,6,7,8] Wibe A. de Jong,[1] Patrick Draper,[9] Aida El-Khadra,[9] Nate Gemelke,[10] Masanori Hanada,[11] Dmitri Kharzeev,[12,13] Henry Lamm,[5] Ying-Ying Li,[5] Junyu Liu,[14,15] Mikhail Lukin,[16] Yannick Meurice,[17] Christopher Monroe,[18,19,20,21] Benjamin Nachman,[1] Guido Pagano,[22] John Preskill,[23] Enrico Rinaldi,[24,25,26] Alessandro Roggero,[27,28] David I. Santiago,[29,30] Martin J. Savage,[31] Irfan Siddiqi,[29,30,32] George Siopsis,[33] David Van Zanten,[5] Nathan Wiebe,[34,35] Yukari Yamauchi,[2] Kübra Yeter-Aydeniz,[36] and Silvia Zorzetti[5]

and many more!

HPC resources, computational hardware and software, partnerships are imperative to achieve our scientific goals

Computational NP and AI/ML Workshop

Computational Nuclear Physics and AI/ML Workshop

Organizers:

- A. Lovato (ANL) • J. Carlson (LANL) • P. Shanahan (MIT)
- B. Messer (ORNL) • W. Nazarewicz (FRIB/MSU) • A. Boehnlein (JLab)
- P. Petreczky (BNL) • R. Edwards (JLab) • D. Dean (JLab)

Participants:

- 60 registered participants including DOE representation

https://indico.jlab.org/event/581/

Tuesday, 6 September

1:00 – 1:05	Welcome, David Dean and Sean Hearne
1:05 – 1:20	DOE remarks, Tim Hallman
1:20 – 2:00	QCD, William Detmold (JLab) and Swagato Mukherjee (BNL)
2:00 – 2:40	Quantum many-body problems, Thomas Papenbrock (UT/ORNL)
2:40 – 3:00	BREAK
3:00 – 3:40	Fundamental Symmetries,Emanuele Mereghetti (LANL)
3:40 – 4:20	Astrophysics, George Fuller (UCSD)
4:20 – 5:00	AI/ML, Amber Boehnlein (JLab)
5:00 – 5:40	Preliminary list of recommendations discussion (Peter Petreczky, lead)
5:40 – 7:30	Reception

Wednesday, 7 September

7:45 – 8:30	Continental Breakfast
8:30 – 10:00	Breakout Sessions 1. QCD (Phiala Shanahan, lead) 2. Nuclear Structure and fundamental symmetries (Alessandro Lovato, lead) 3. Astrophysics (Bronson Messer, lead)
10:00 – 10:30	Break
10:30 – 12:00	Breakout reports
12:00 – 1:00	Lunch
1:00 – 2:30	Recommendations discussion and next steps

Jefferson Lab Thomas Jefferson National Accelerator Facility

SURA

Deliverable: white paper for LRP

Workshop resolution

High-performance computing is essential to advance nuclear physics on the experimental and theory frontiers. Increased investments in computational nuclear physics will facilitate discoveries and capitalize on previous progress. Thus, we recommend a targeted program to ensure the utilization of ever-evolving HPC hardware via software and algorithmic development, which includes taking advantage of novel capabilities offered by AI/ML.

The key elements of this program are to:

1) Strengthen and expand programs and partnerships to support immediate needs in HPC and AI/ML, and also to target development of emerging technologies, such as quantum computing, and other opportunities.

2) Take full advantage of exciting possibilities offered by new hardware and software and AI/ML within the nuclear physics community through educational and training activities.

3) Establish programs to support cutting-edge developments of a multi-disciplinary workforce and cross-disciplinary collaborations in high-performance computing and AI/ML.

4) Expand access to computational hardware through dedicated and high-performance computing resources.

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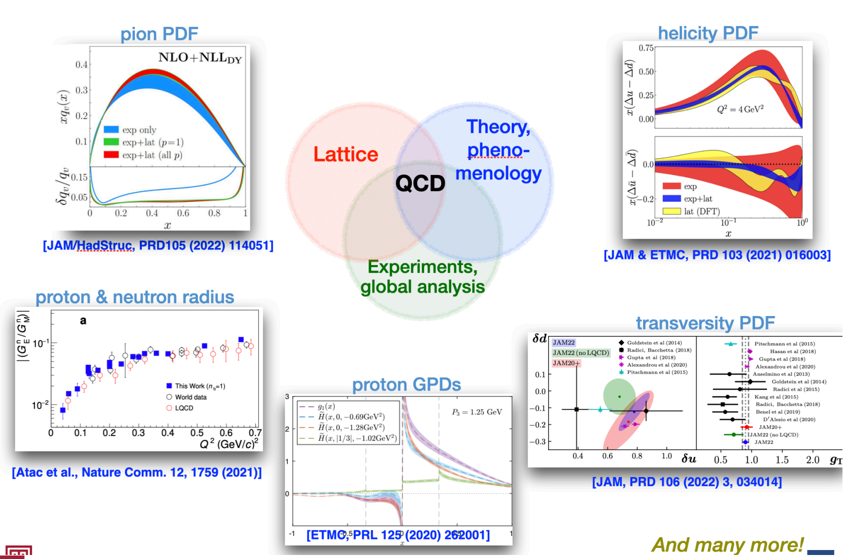
Many opportunities for synergies and complementarity.

But perhaps the best way to understand its full capabilities is to imagine for a moment the impact of taking it away.

Synergies: constraints & predictive power of lattice QCD



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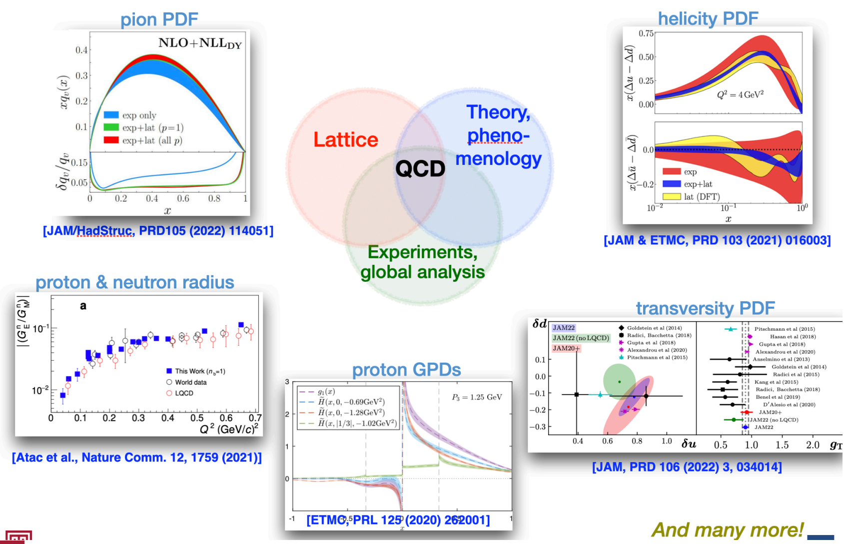

And many more!

Thank you