



Nuclear Science Long Range Plan and Computing

26th International Conference on Computing in High-Energy & Nuclear Physics (CHEP2023)

Haiyan Gao, Nuclear and Particle Physics, BNL

May 10, 2023



@BrookhavenLab

Acknowledgment

Thank all DNP Town Meeting conveners

Leah Broussard, Vincenzo Cirigliano, Jon Engel, Alex Gade, Sofia Quaqlioni, Grigory Rogachev, Bjoern Schenke, Anne Sickles, Rebecca Surman, Lindley Winslow, Feng Yuan, Xiaochao Zheng for organizing these successful meetings, the community whitepapers and their help with this presentation.

And

Amber Boehnlein, Giordano Cerizza, Kelly Chipps, David Dean, Jason Detwiler, Jon Engel, Julieta Gruszko, Eric Lancon, Dean Lee, Swagato Mukherjee, Amy Nicholson, Peter Petreczky, Bob Tribble, John Wilkerson for their help with this presentation

Monday's keynotes by David Dean and Markus Diefenthaler covered Computing and future trends in NP computing very well and thank you!

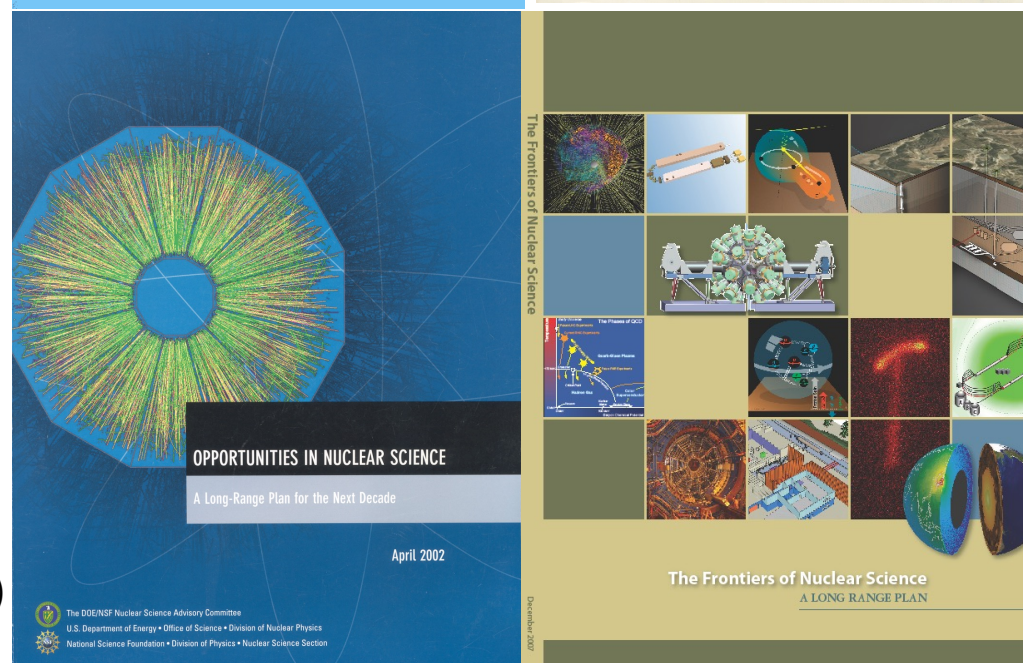
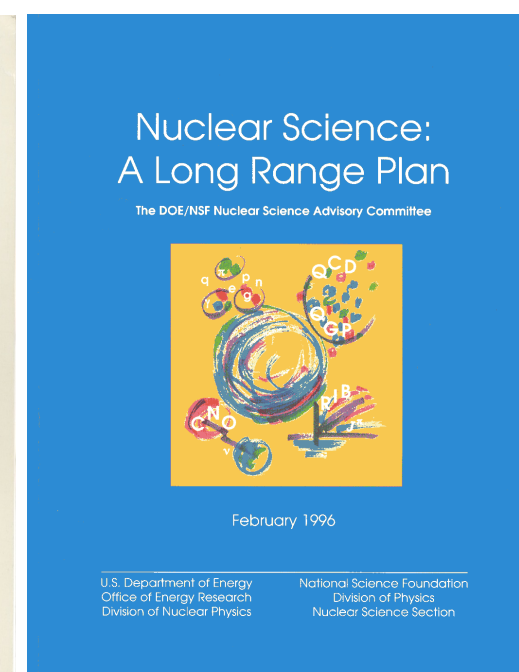
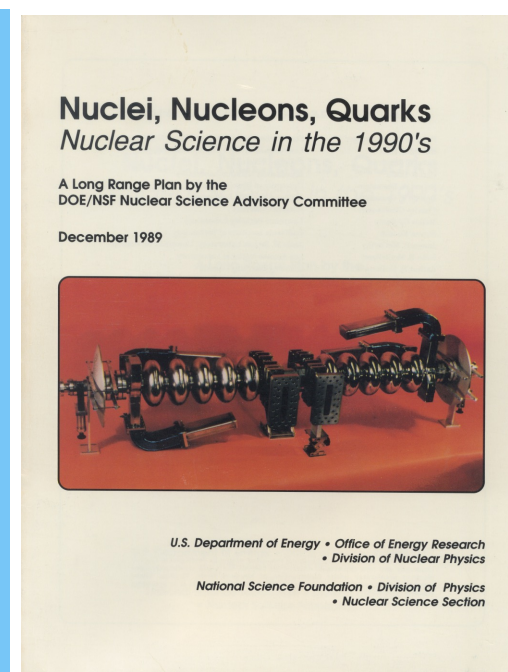
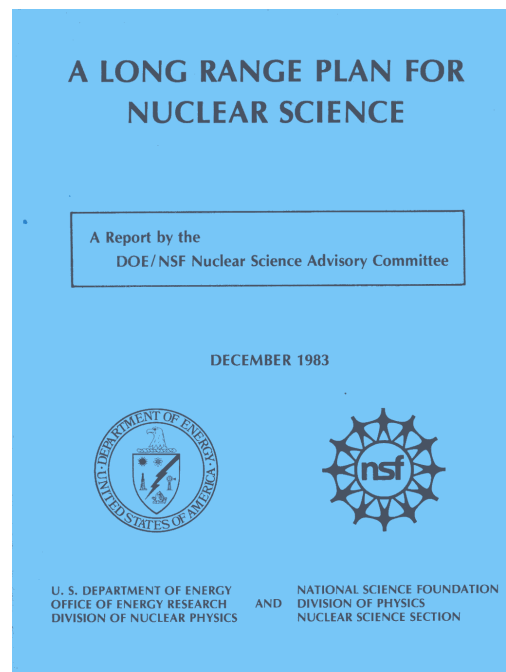
Brookhaven National Laboratory is supported by the U.S. Department of Energy's Office of Science.

DOE and NSF formed NSAC in 1977

TABLE II
NUCLEAR SCIENCE FACILITY CONSTRUCTION PLAN

	FISCAL YEAR	80	81	82	83	84	85	86	87	88	89
PRIOR	Bevalac Uranium	\$4M	1								
	Michigan State Phase 2	6	8	8	5						
	Bates Energy Doubler and Pion Spectrometer	3									
	LAMPF Staging Area	2.4									
	Stony Brook, Caltech	2	1								
	Argonne Atlas	6									
NEW	Neutrino Horn LAMPF			2							
	Light-Heavy Upgrade 1			7							
	Heavy Ion Upgrade				7						
	Kaon channel				7						
	CW electron accel. (medium energy) Illinois/Stanford			3							
	Nuclear theory computer					12					
	High Energy Light Ion upg.						10				
	Light or Heavy Ion upg. 2					7					
	High Energy CW Electron Accel. 1-2 GeV						10	20	20		
	Upgrade									7	
	Upgrade									7	
	User Facility									5	13
	Upgrade										7
TOTAL		17.4	16	20	19	19	20	20	20	19	20

- 1979 LRP (~30 people @ meeting, recommendations in table)
 - 1983 LRP (J. Schiffer)
 - 1989 LRP (P. Paul)
 - 1996 LRP (E. Moniz/H. Robertson)
 - 2002 LRP (J. Symons)
 - 2007 LRP (R. Tribble)
 - 2015 LRP (D. Geesaman)
 - 2023 LRP ongoing (G. Dodge)
- (town meetings: ~1300, ~600 (in person))



DOE/NSF Charge for NSAC

The new NSAC LRP should articulate the scope and the scientific challenges of nuclear physics today, what progress has been made since the last LRP, and the impacts of these accomplishments both within and outside the field. It should identify and prioritize the most compelling scientific opportunities for the U.S. nuclear physics program to pursue over the next decade (fiscal year (FY) 2023-2032) and articulate its potential scientific impact. Further, a nationally coordinated strategy for the use of existing and planned capabilities, both domestic and international, and the rationale for new investments should be articulated. To be most helpful, the LRP should indicate what resources and

Town Hall Meetings (led by Division of Nuclear Physics, APS)
are part of the NSAC LRP exercise:

- Nuclear structure, reactions & astrophysics, ANL, Nov. 14-16, 2022
- Fundamental symmetries, neutrons, neutrinos, UNC Chapel Hill, Dec. 14-16, 2022
- Hot and Cold QCD, MIT, Sept. 23-25, 2022

578 Participants
216 in person
362 remote

Co-Conveners: Alex Gade, Sofia Quaglioni,
Grigory Rogachev, Rebecca Surman
Local Organization co-Chairs: Ben Kay, Mike Carpenter



*NSAC Long Range Plan Town Hall Meeting on Nuclear Structure, Reactions, and Astrophysics
November 14-16, 2022*

Next decade intellectual challenges for nuclear structure, reactions and astrophysics captured in new questions

What is the nature of the nuclear force that binds protons and neutrons into stable nuclei and rare isotopes, and how do the rich phenomena of nuclear structure and reactions emerge?

How do single-nucleon, cluster, and collective degrees of freedom coexist and evolve with increasing proton-neutron imbalance and excitation energies?

What are the limits of nuclear existence, and what features arise near and beyond these limits?

What are the astrophysical origins of the elements and how did the associated chemical evolution proceed?

How do stars evolve, and what nuclear signatures do they leave behind?

What is the nature of neutron stars and dense matter?

How can the knowledge and technological progress provided by nuclear science best be used to benefit society?

https://indico.phy.anl.gov/event/22/attachments/72/393/TownMeeting_Whitepaper_StructureReactionsAstro.pdf

To answer these questions: research program in nuclear structure, reactions, astrophysics with experiment+theory working in concert

Arrive at a predictive understanding of atomic nuclei and their decays and reactions

Chart the limits of nuclear existence

Provide accessible, state-of-the-art, accredited nuclear data to advance nuclear science and its broad applications



Reveal the underlying nuclear physics of stars, stellar explosions, and element synthesis in the cosmos

Apply nuclear science for societal benefit

Leverage the properties of nuclei to enable precision tests of nature's fundamental symmetries



Computing from Nuclear structure, reactions & astrophysics

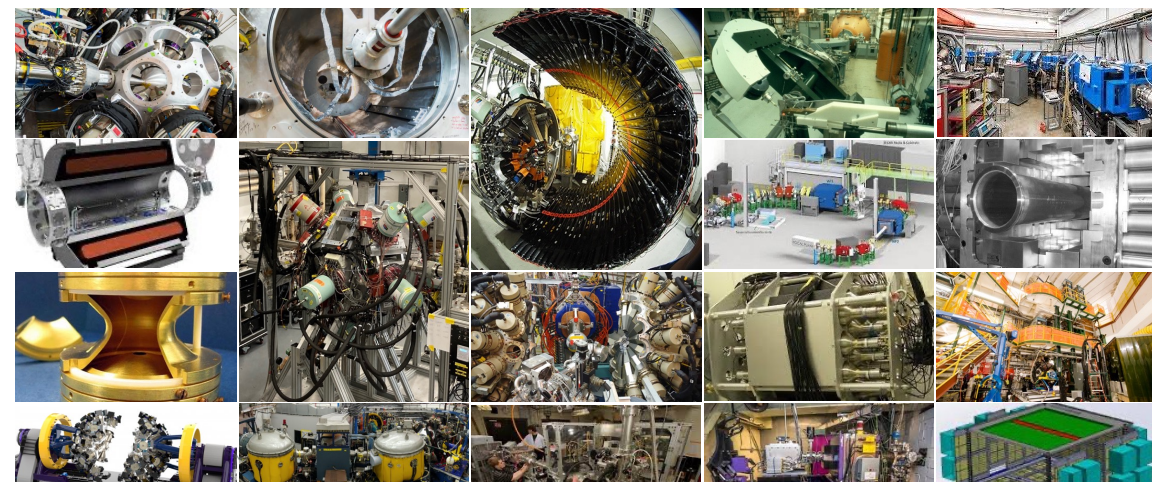
HPC at the Exascale

Predictive capabilities:

- Structure & reactions of light nuclei
- Nuclear matrix elements
- Neutrino & electron int.
- Nuclear matter; Fission
- Nucleosynth., explosions

AI/ML

- UQ, extrap. in structure, reactions, astrophysics
- Fast, accurate emulators
- Experiment design
- Detect. design, particle id, beam tuning, upgrades
- ML for 'multi-setup' data
- Training of large models



QC

- Ideal for many-body syst.
- Solve NP problems with known 'classical' issues
- Algorithms & demos: state prep; time evol.; spectral density
- Guide QC hardware design

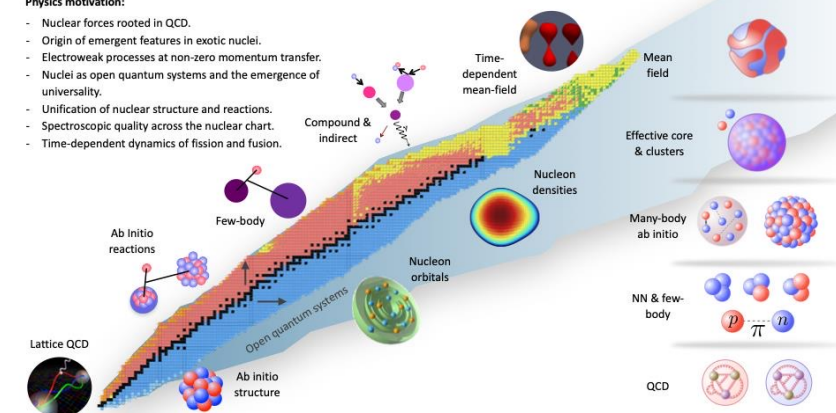
Needs

- Support for refactoring/optimizing codes
- Increased access: Capacity, HPC, many-core (GPUs, tensor proc. units) computer resources
- Interdisciplinary Collabs: Math, CS; AI/ML; QIS



Physics motivation:

- Nuclear forces rooted in QCD.
- Origin of emergent features in exotic nuclei.
- Electroweak processes at non-zero momentum transfer.
- Nuclei as open quantum systems and the emergence of universality.
- Unification of nuclear structure and reactions.
- Spectroscopic quality across the nuclear chart.
- Time-dependent dynamics of fission and fusion.



Computational Issues for the FRIB Scientific Experimental Program

- Define environments that can scale from simple desktop machines to HPC systems.
- Compatibility with legacy software.
- Ability to extend to any number and type of auxiliary detectors from different universities or national laboratories.
- Ability to readout data in trigger-less mode to bypass issues as event pile-up or overlapping of signals from different events.
- Ability to analyze data at 100x incoming rate to support decision making in real time.
- Taking advantage of AI/ML for tasks such as automatic beam tuning, particle identification, event reconstruction and classification...

Report from the “Fundamental Symmetries, Neutrons and Neutrinos” Town Hall

Vincenzo Cirigliano

University of Washington



Co-Conveners:

Leah Broussard (ORNL), Jon Engel (UNC), Lindley Winslow (MIT)

275 participants, of which ~ 180 in person
December 13-15, 2022

APS April Meeting
April 16 2023, Minneapolis

Fundamental Symmetries, Neutrons, and Neutrinos (FSNN):

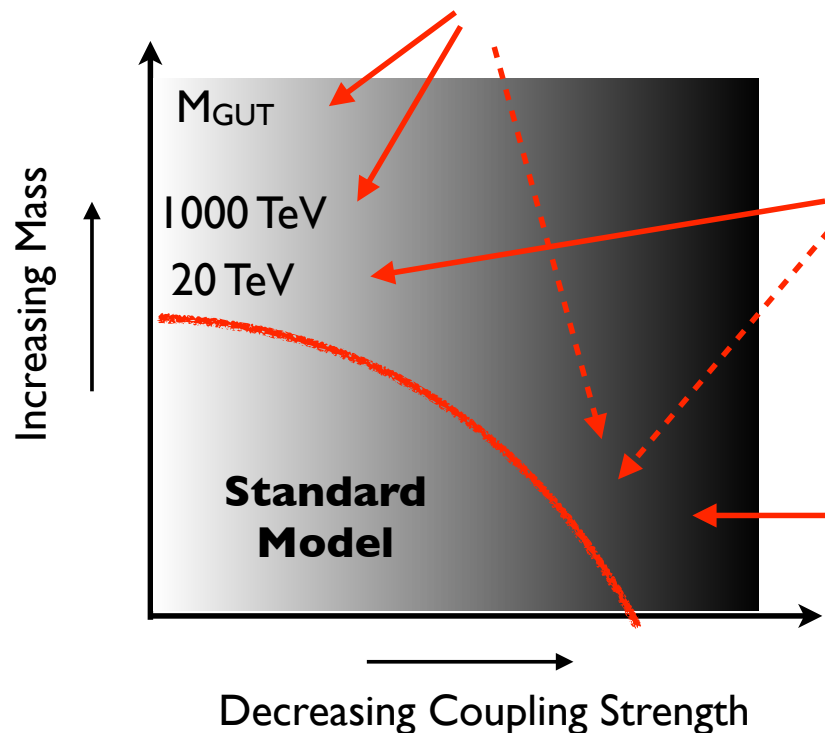
Whitepaper for the 2023 NSAC Long Range Plan

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Nuclear Science FSNN portfolio

- Three classes of low-energy probes, pushing the boundary of BSM sensitivity in qualitatively different ways and at different mass scales

1. **Searches for rare or SM-forbidden processes** that probe approximate or exact symmetries of the SM (L, B, CP, L_α): $0\nu\beta\beta$ decay, EDMs, n - $\bar{n}$ oscillations, $\mu \rightarrow e$ conversion, $e p \rightarrow \tau X$, ...



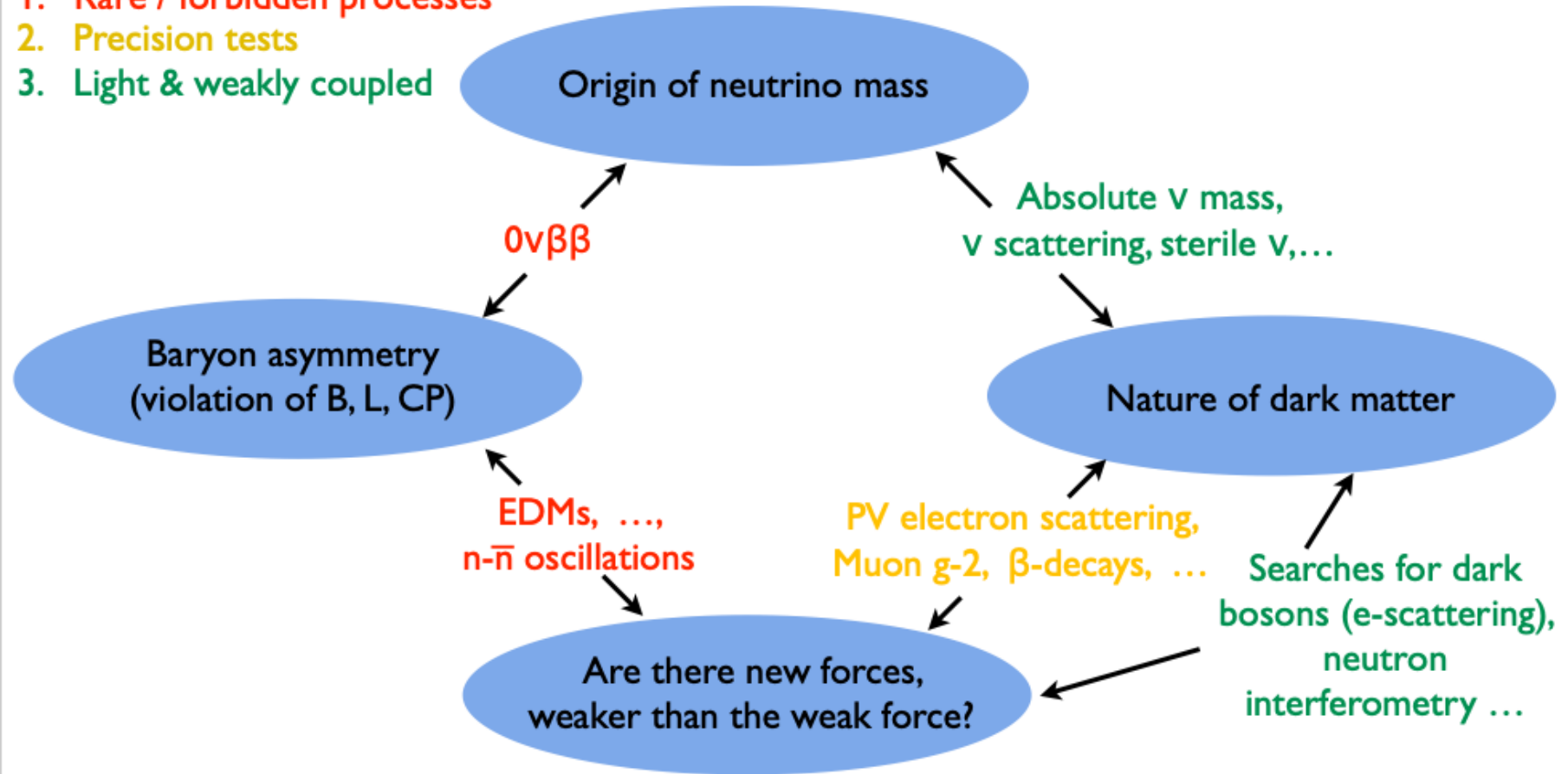
2. **Precision tests** of SM-allowed processes: β -decays (mesons, neutron, nuclei), muon $g-2$, PV electron scattering, HPV, ...

3. Searches / characterization of **light and weakly coupled particles**: active ν 's, sterile ν 's, dark sector particles and mediators, axions, ...

Shedding light on big questions

FSNN probes cluster around four interconnected questions

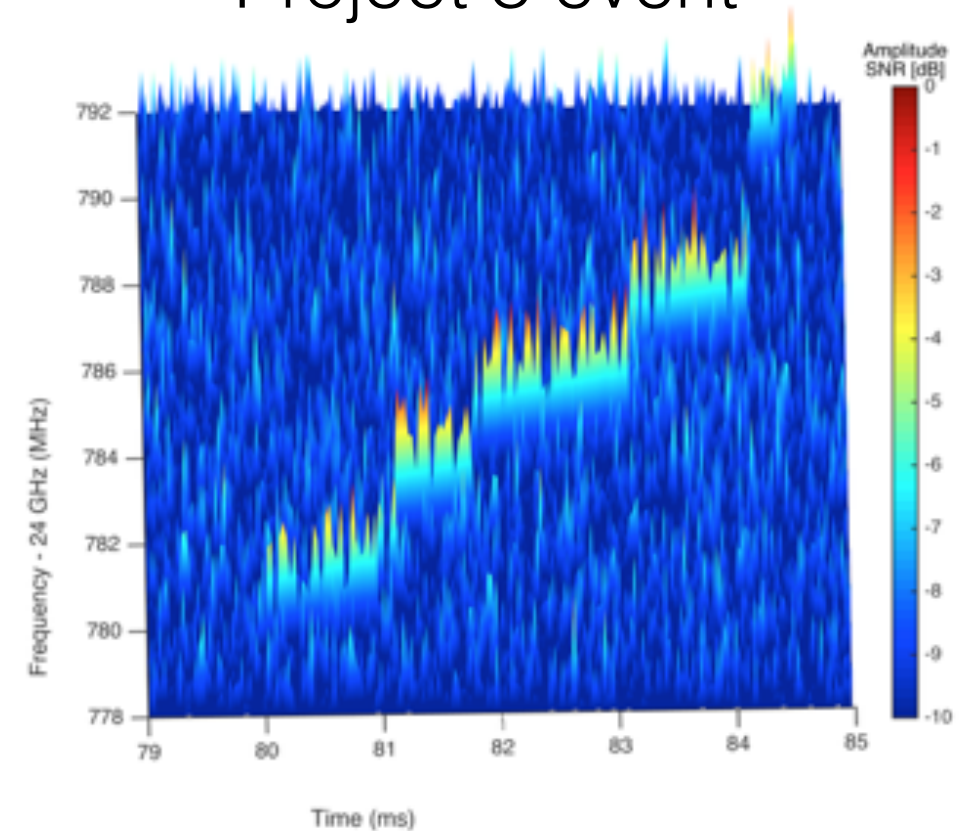
1. Rare / forbidden processes
2. Precision tests
3. Light & weakly coupled



Key Computational Challenges for FSNN

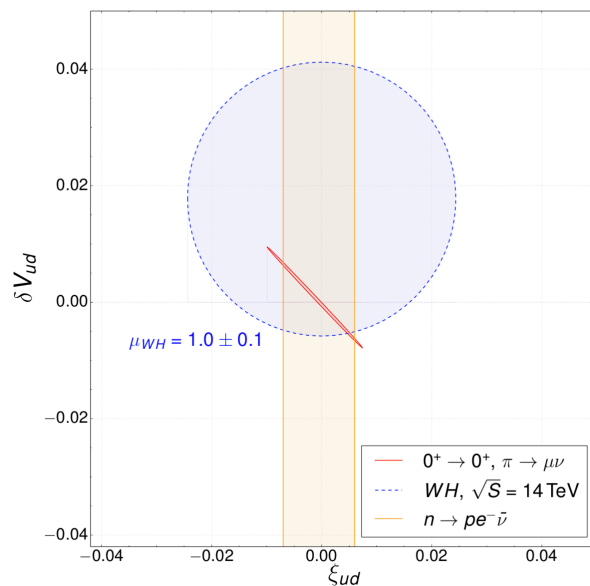
- Exposure-limited sensitivity: precious data
 - All data on disk
 - Optimization → reprocessing
 - Remote access
- Few groups make use of massive parallelism at present
- Many groups not associated with a major facility
- If anyone sees a BSM signal, theorists are suddenly going to need a lot more computing.
- **Project 8:** Cyclotron Radiation Emission Spectroscopy
 - RF time series recorded at 100 MB/s per receiver (~3 PB/yr)
 - Locate tracks and measure energy, pitch, other topology info (FFT, DBSCAN, Consensus Thresholding, KD-Trees, Hough Transforms...)
 - Current: 1 receiver, short runs: TB of data, hundreds of kCPU-hrs processing, little parallelism.
 - Future: 60 receivers, longer runs → ~200 PB/yr, millions of CPU-hrs. Data reduction and GPU methods under investigation.

Project 8 event



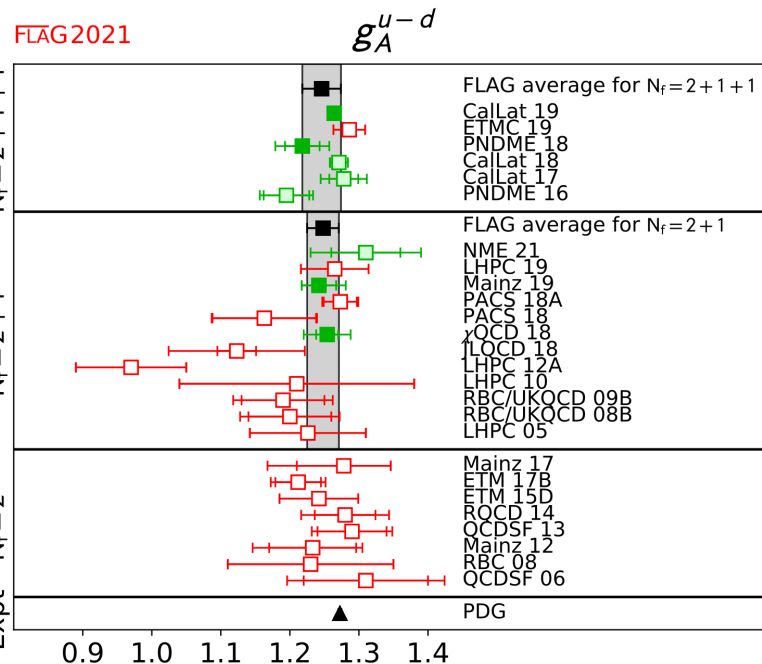
Jason Detwiler





**LQCD + neutron decay
now places tightest
constraints on right-
handed BSM currents**

Adapted from: Alioli, S.,
Cirigliano, V., Dekens, W.,
de Vries, J., and Mereghetti, E.
JHEP 05, 086 (2017)



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Letter | Published: 30 May 2018

A per-cent-level determination of the nucleon axial coupling from quantum chromodynamics

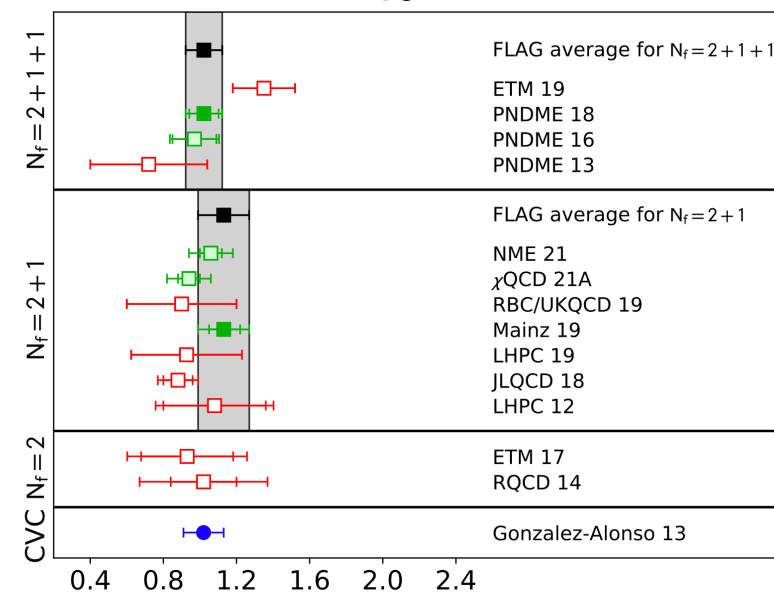
C. C. Chang, A. N. Nicholson, E. Rinaldi, E. Berkowitz, N. Garron, D. A. Brantley, H. Monge-Camacho, C. J. Monahan, C. Bouchard, M. A. Clark, B. Joó, T. Kurth, K. Orginos, P. Vranas & A. Walker-Loud

Nature 558, 91–94 (2018) | Cite this article

4101 Accesses | 109 Citations | 129 Altmetric | Metrics

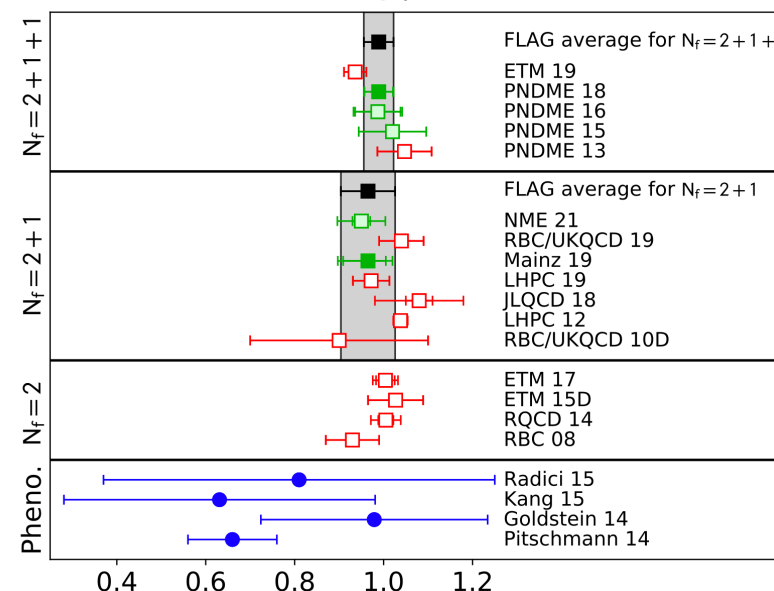
FLAG2021

g_S^{u-d}



FLAG2021

g_T^{u-d}



Hot and Cold QCD Town Meeting, September 23-25, 2022, MIT

Ian Cloët (ANL)

Or Hen (MIT)

David Lawrence (JLab)

Wei Li (Rice)

Swagato Mukherjee (BNL)

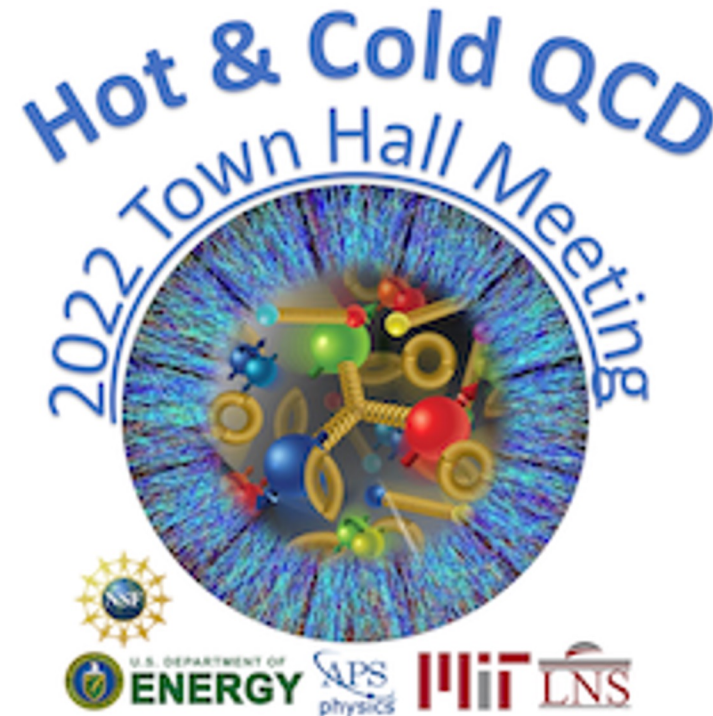
Bjoern Schenke (BNL)

Anne Sickles (Illinois)

Ramona Vogt (LLNL & UCD)

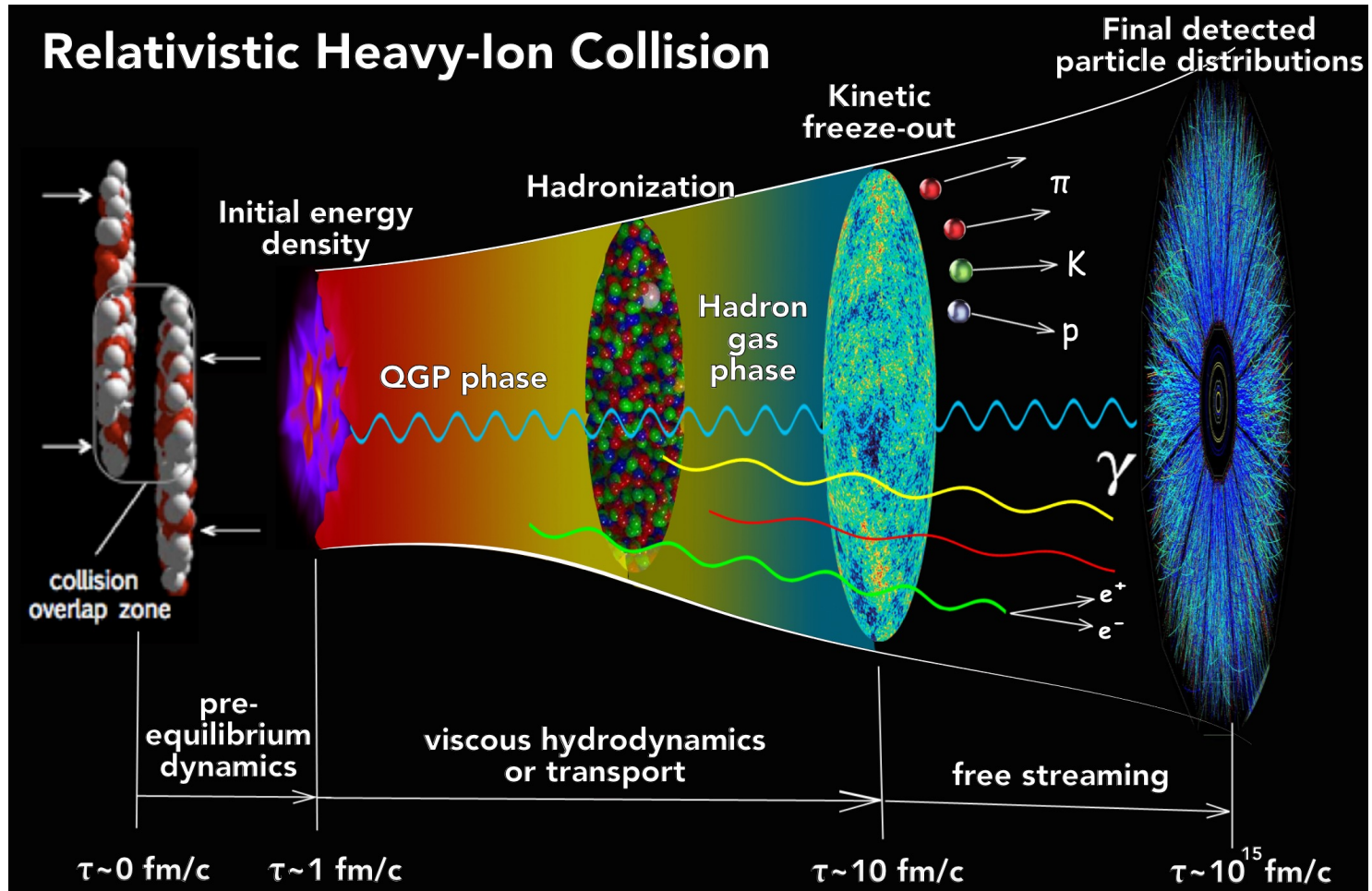
Feng Yuan (LBNL)

Xiaochao Zheng (UVA)



<https://indico.mit.edu/event/538/>

Probing the hot QCD



Hard: Jet, heavy flavor, ...
Soft: anisotropy (v_n),
correlations, fluctuations, ...
EM: photon, dilepton, ...

Experiments:
Relativistic Heavy Ion Collider
(RHIC) @ BNL; Large
Hadron Collider (LHC) @
CERN

CBM@FAIR

Cold QCD: from quark to cosmos

How do the spin and orbital degrees of freedom of quarks and gluons within the nucleon combine to make up its total spin?

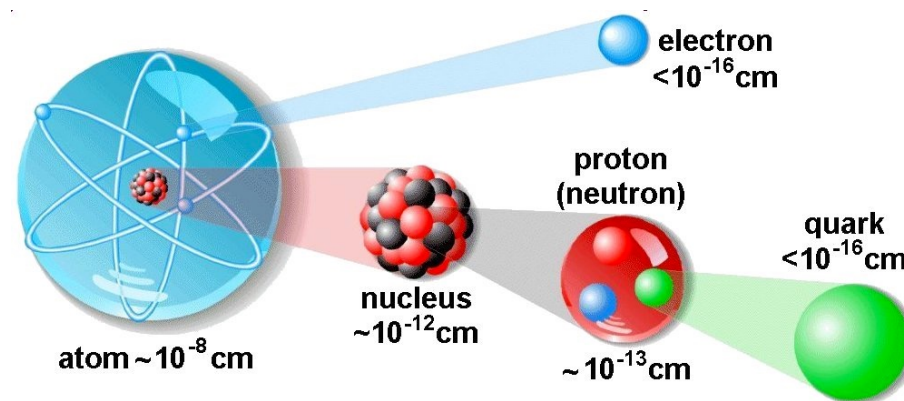
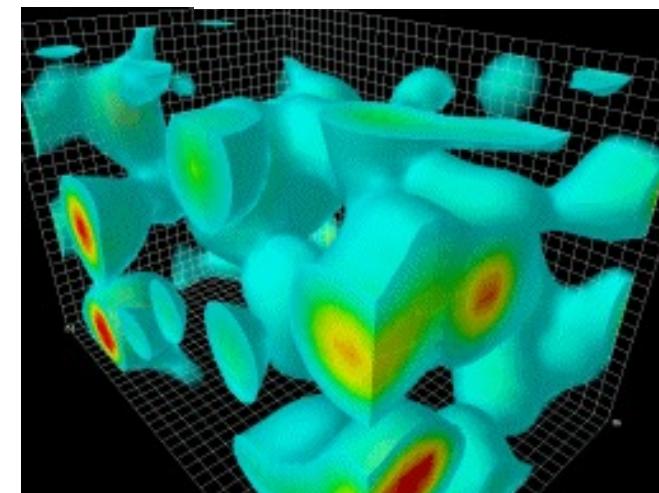
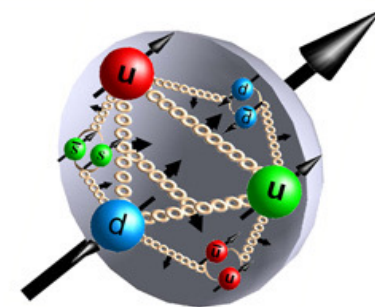
What is the origin of the mass of the nucleon and other hadrons?

Do gravitational form factors inform us about the origin of mass and can they be extracted from measurements?

Where are the quarks and gluons located within the nucleon?

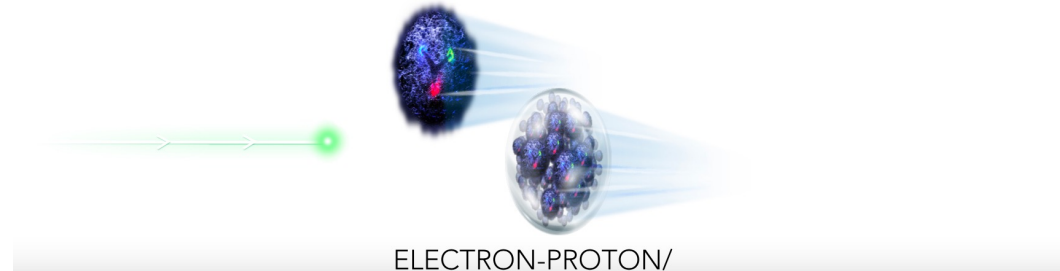
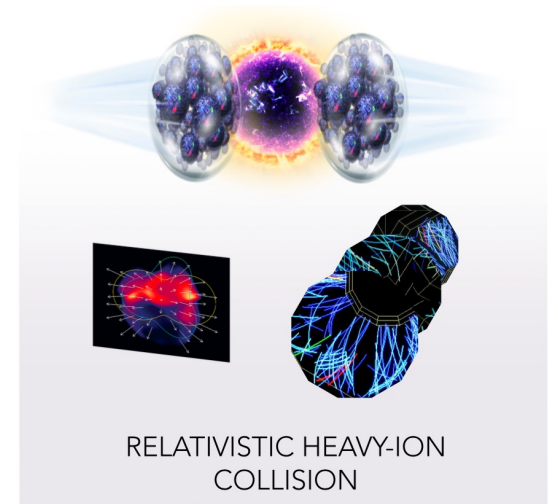
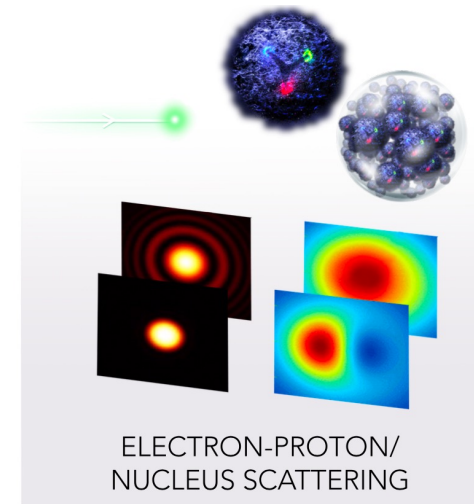
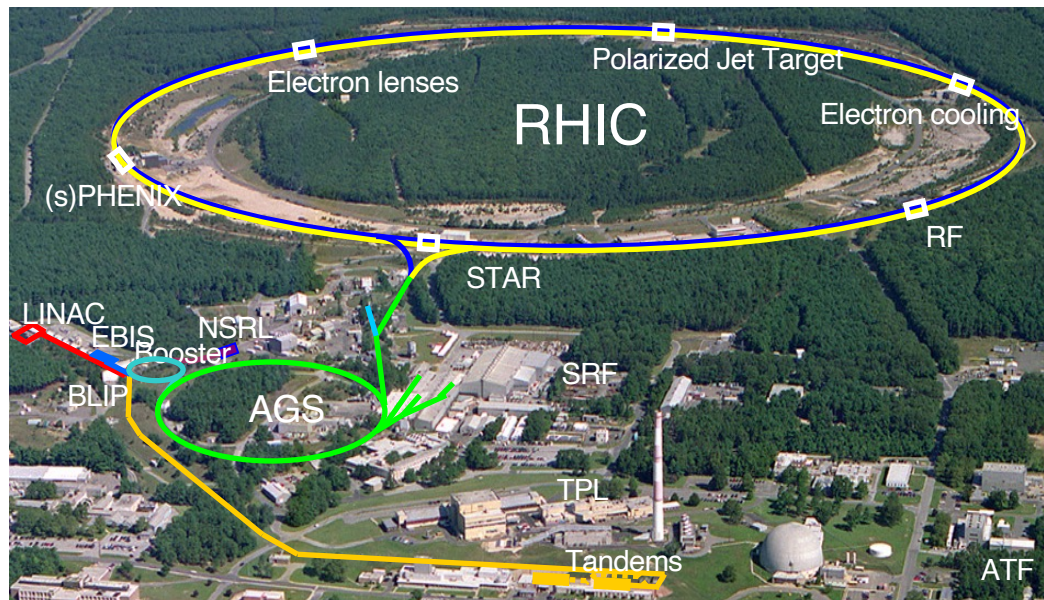
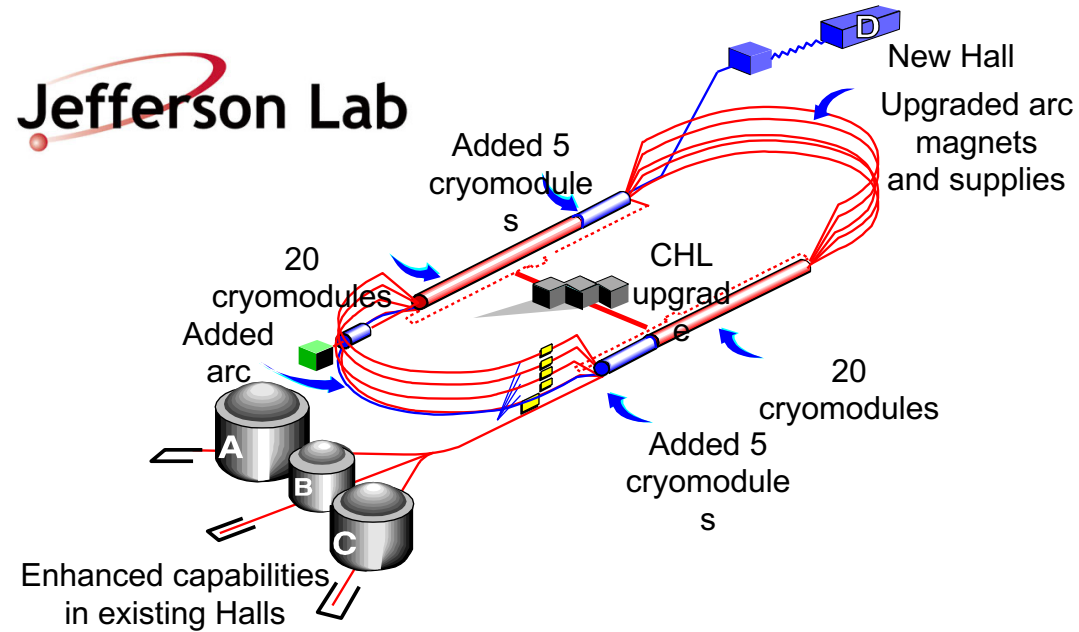
How does the quark-gluon structure of the nucleon change when it is bound in the nucleus?

What is the spectrum and structure of conventional and exotic hadrons?



Current major DOE QCD facilities

Jefferson Lab



2022: Joint effort from both hot and cold QCD

[QCD White Paper](#)

<https://arxiv.org/abs/2303.02579>

The Electron-Ion Collider

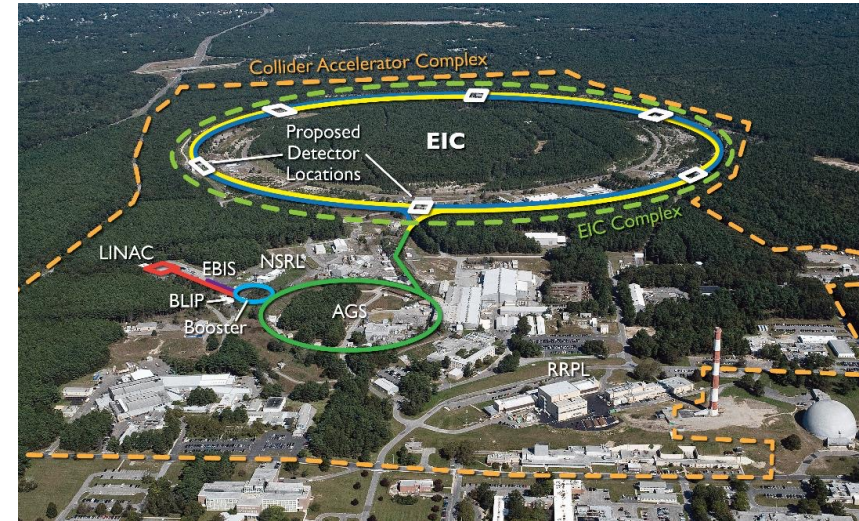
2015 NSAC LRP

"We recommend a high-energy high-luminosity polarized EIC as the highest priority for new facility construction following the completion of FRIB."

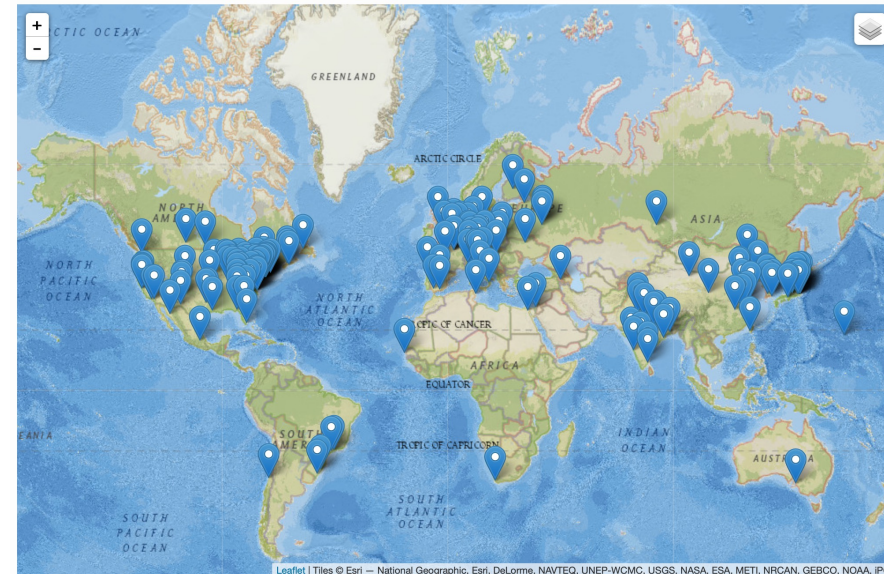
Project Design Goals

- High Luminosity: $L = 10^{33} - 10^{34} \text{ cm}^{-2} \text{ sec}^{-1}$, $10 - 100 \text{ fb}^{-1}/\text{year}$
- Highly Polarized Beams: $\sim 70\%$
- Large Center of Mass Energy Range: $E_{\text{cm}} = 20 - 140 \text{ GeV}$
- Large Ion Species Range: protons – Uranium
- Large Detector Acceptance and Good Background Conditions
- Accommodate a Second Interaction Region (IR)

Conceptual design scope and expected performance meet or exceed NSAC Long Range Plan (2015) and the EIC White Paper requirements endorsed by NAS (2018)



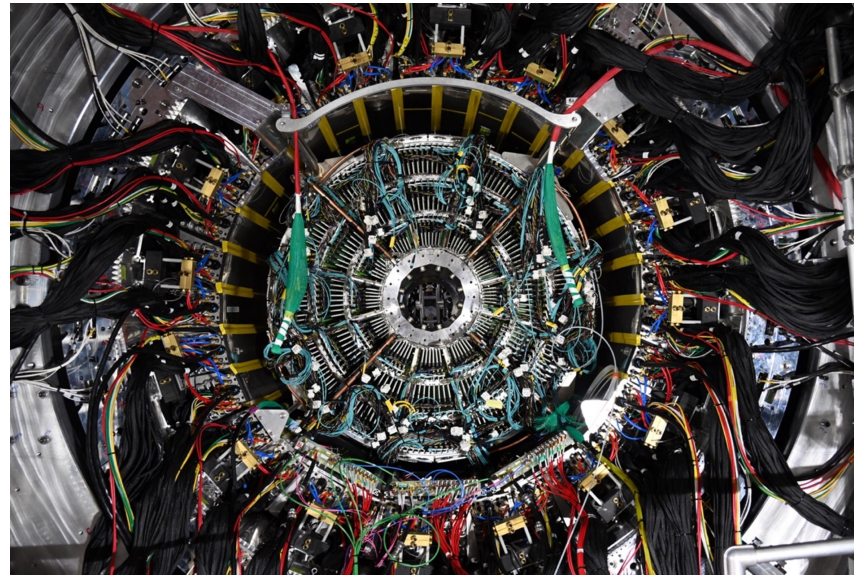
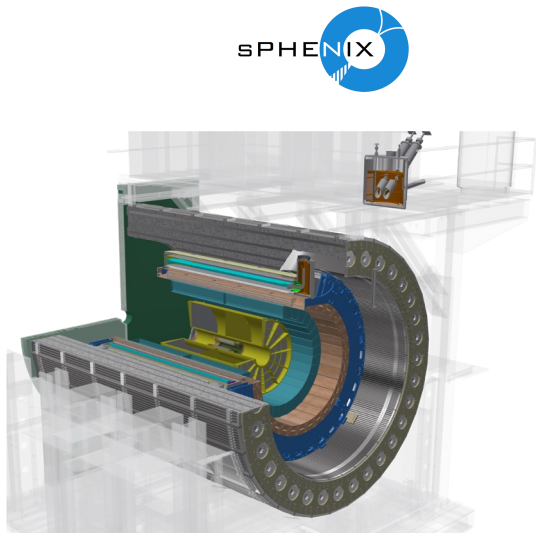
Double Ring Design Based on Existing RHIC Facility



1362 collaborators, 36 countries, 267 institutions

Complete RHIC Science Mission in 2015 NSAC LRP

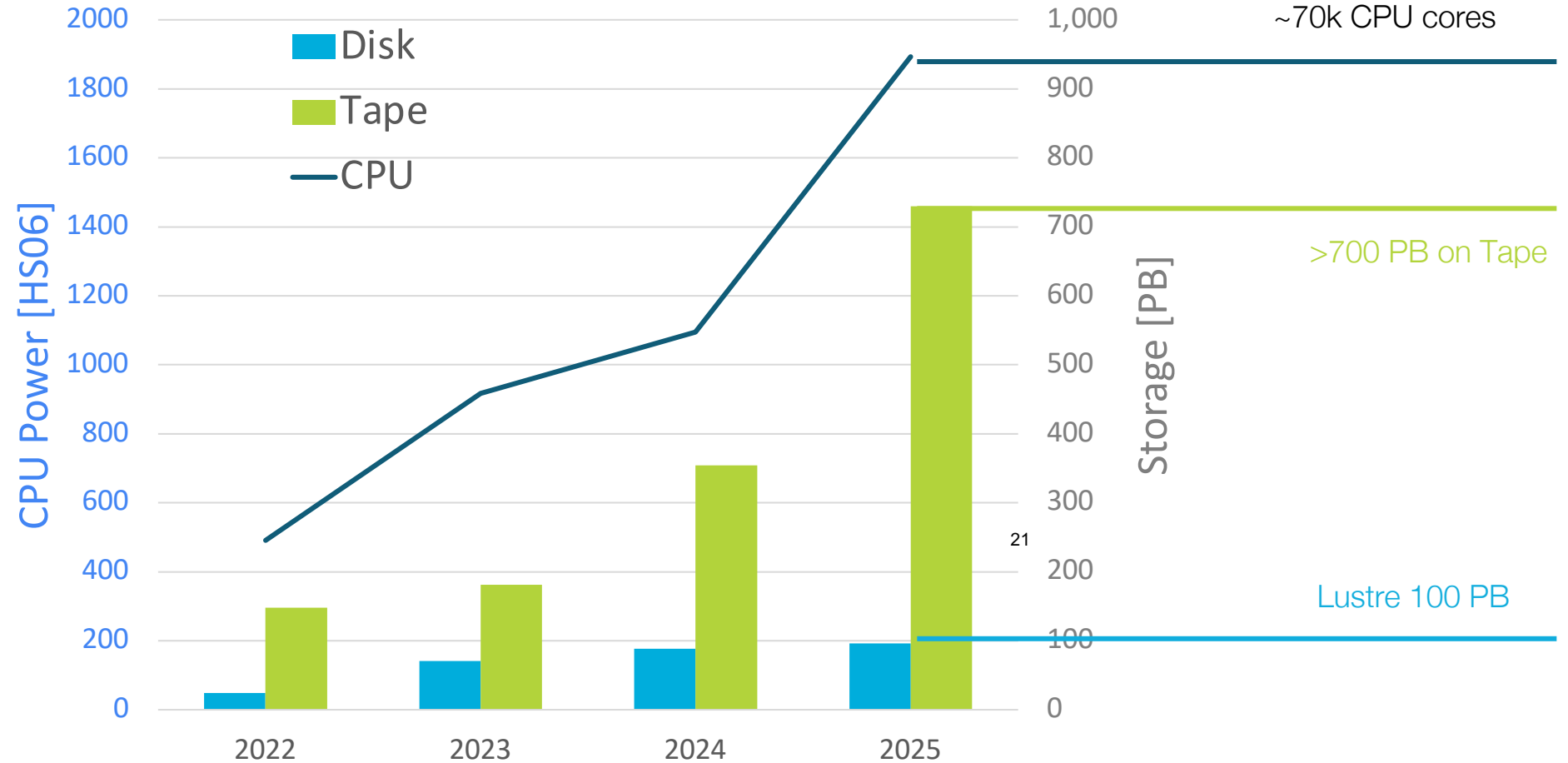
- sPHENIX will use energetic probes (jets, heavy quarks) to study quark-gluon plasma with unprecedented precision
- How the structureless "perfect" fluid emerges from the underlying interactions of quarks and gluons at high temperature



RHIC data taking scheduled for 2023–2025
sPHENIX upgrade and STAR with forward upgrade will fully utilize the enhanced (~ 50 times Au+Au design) luminosity of RHIC

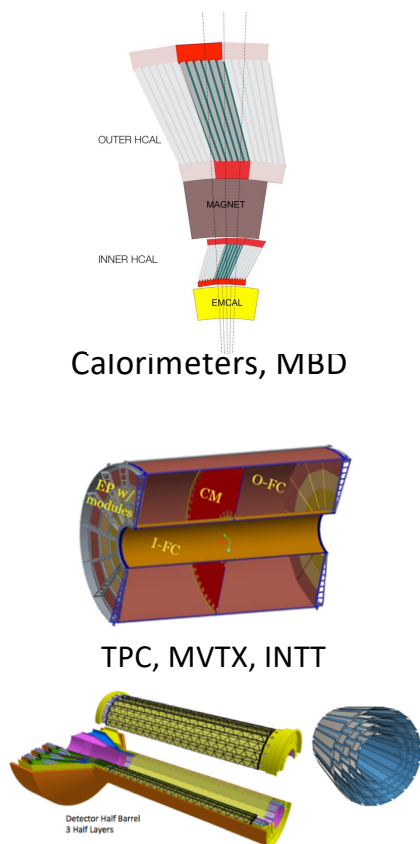
RHIC computing evolution

4-6 increase
over the
next 3 years

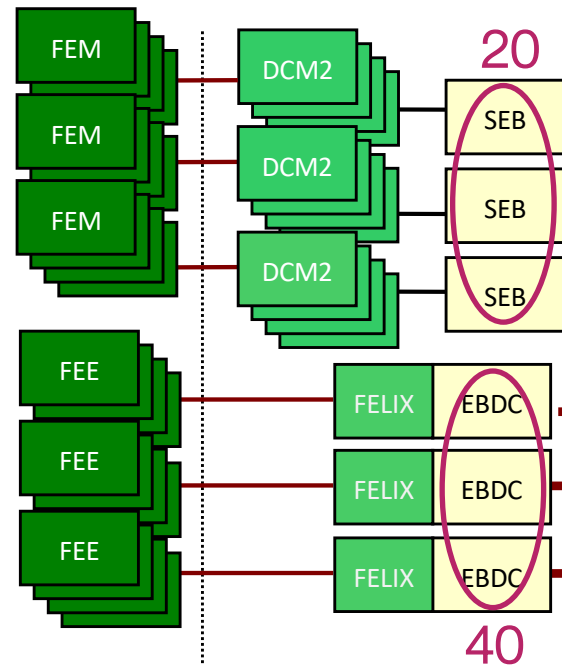


sPHENIX

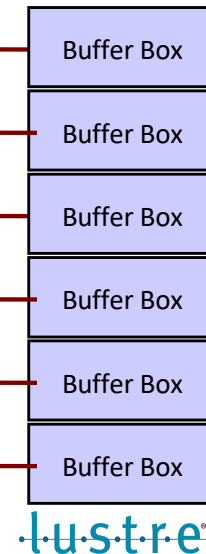
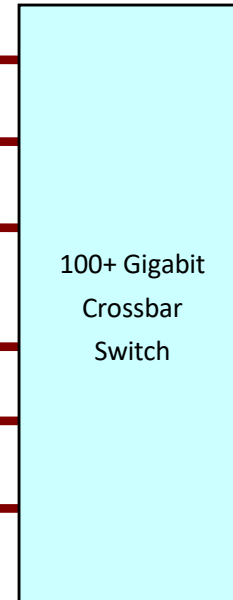
Data Streaming and nearline processing



Trigger readout

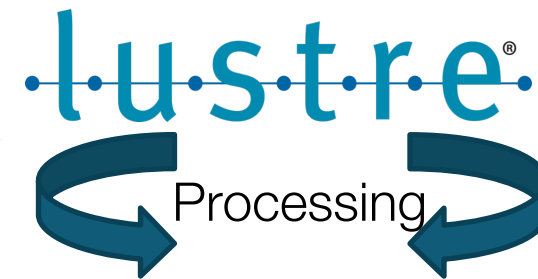


Streaming readout



10 GB/s

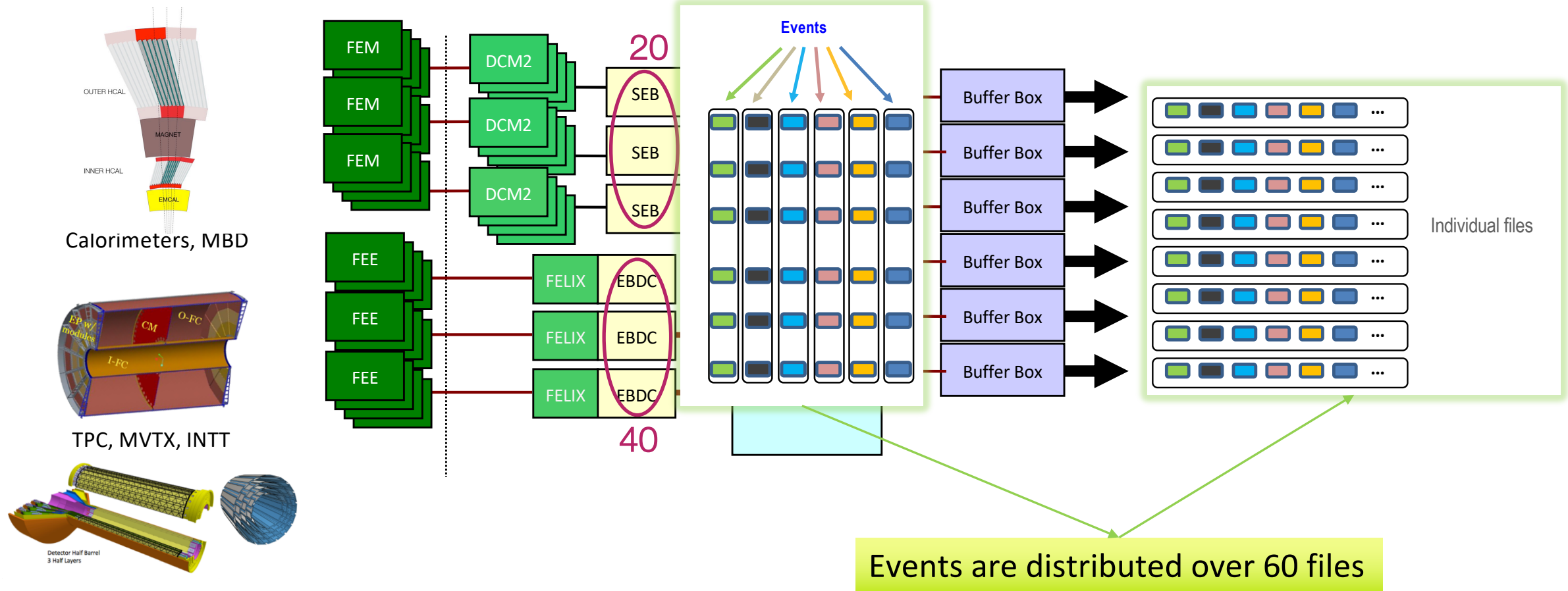
Archive



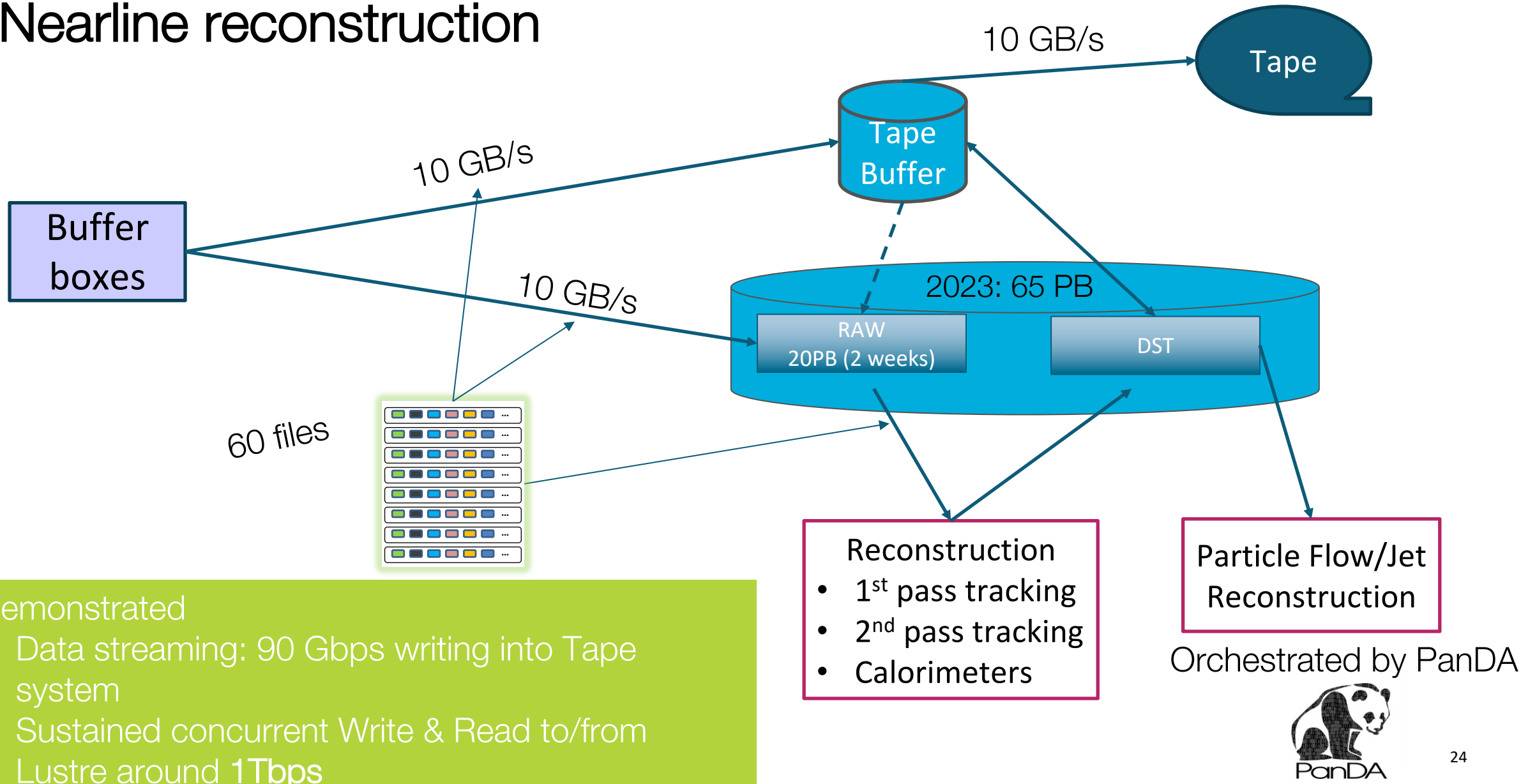
FEM/FEE: Front-End Module / Electronics
 DCM2 - Data collection Module (v2)
 FELIX - ATLAS-developed readout card
 SEB - SubEvent Buffer
 EBDC - Event Buffer and Data Compressor

sPHENIX

Data Streaming and nearline processing



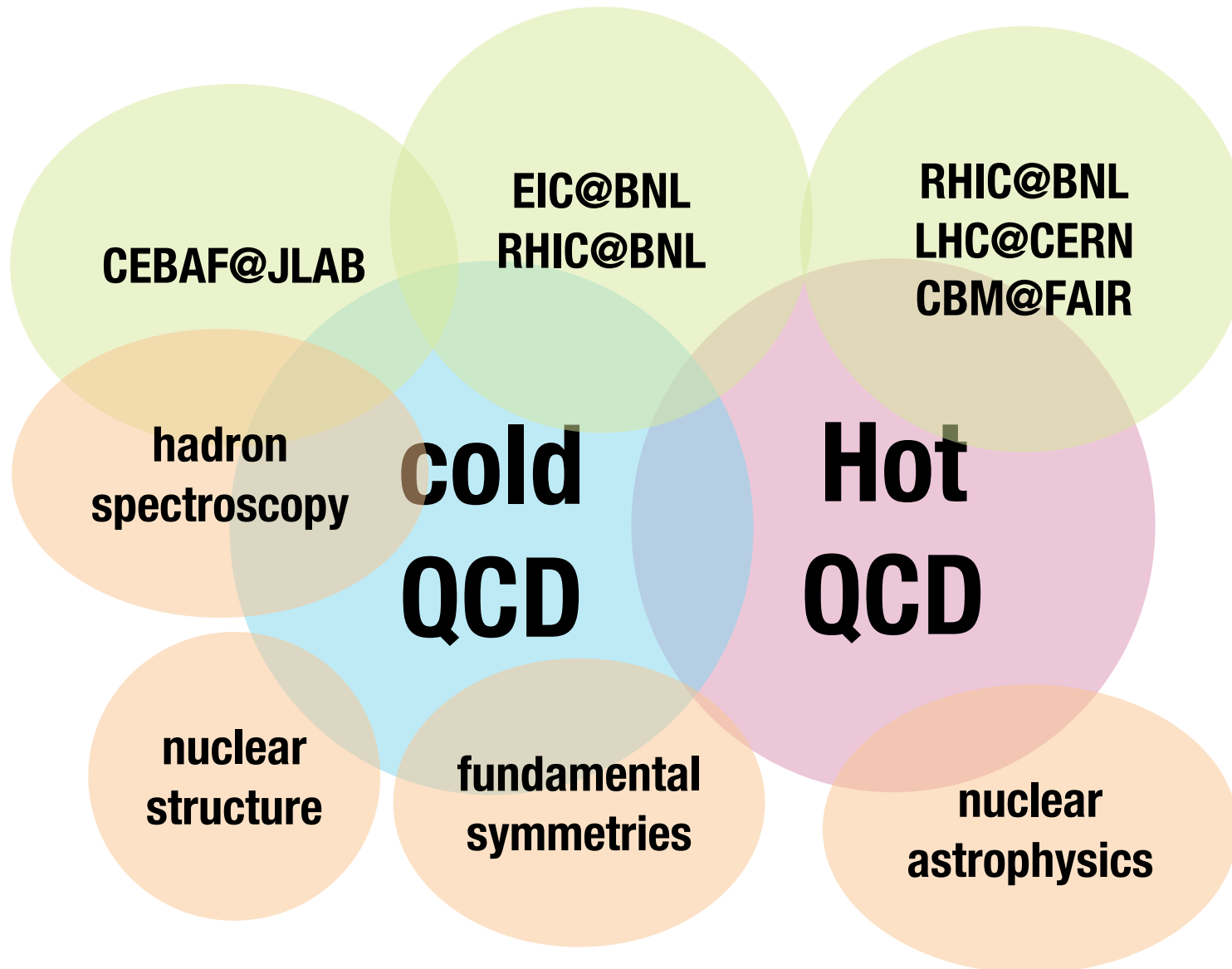
Nearline reconstruction



Demonstrated

- Data streaming: 90 Gbps writing into Tape system
- Sustained concurrent Write & Read to/from Lustre around 1Tbps

Lattice QCD calculations will impact all of US Nuclear Physics Program



Essential for progress:

- Access to Leadership Class Computing Facilities, e.g. ALCF, OLCF through programs like ALCC and INCITE as well as NERSC and dedicated computing resources of USQCD

USQCD provides test bed of new hardware
21g cluster first cluster with AMD GPUs
⇒ Frontier at OLCF equipped with AMD GPUs

- Development of highly specialized and optimized software for lattice QCD ?

SiCDAC-3: 2012-2017
SciDAC-4: 2017-2022
SciDAC-5: 2023-2028
??? 2028-

Hot lattice QCD long range plan

- ◉ sPHENIX, LHC: state-of-the-art lattice QCD results for heavy quarks in quark gluon plasma
 - ◉ heavy quark diffusion coefficient
 - ◉ thermal masses, widths of quarkonia
 - ◉ complex static quark potential

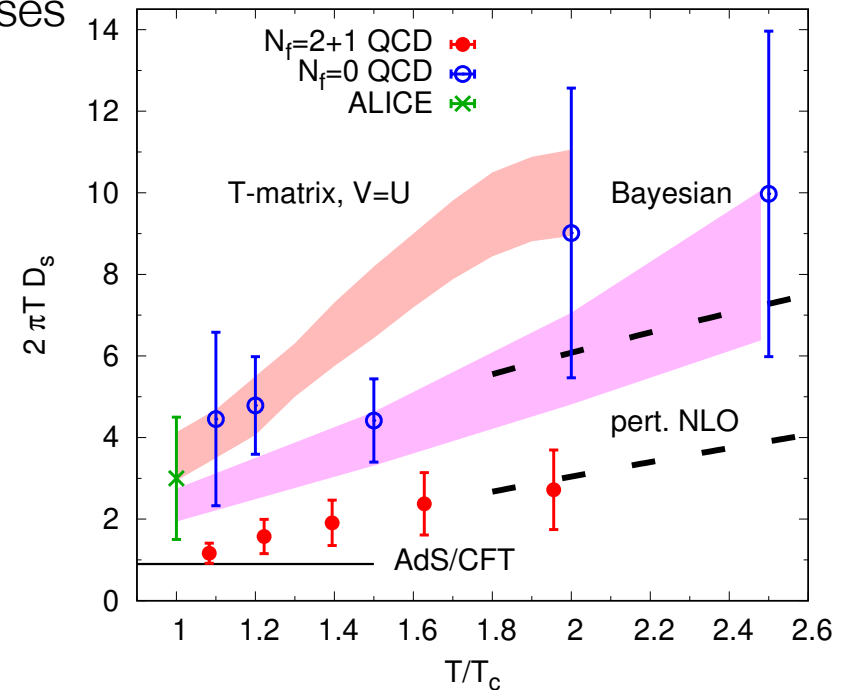
These quantities are encoded in spectral functions

⇒ difficult inverse problem

⇒ very small lattice spacings

Algorithmic
developments
Exa-scale computing
resources are needed

First lattice QCD calculations: small lattice spacing but unphysical quark masses



- ◉ Theory support for RHIC BES-2 program and CBM: extend the reach of lattice QCD calculations to larger μ_B

Cold QCD: hadron structure

how properties of existing matter arise from QCD ?

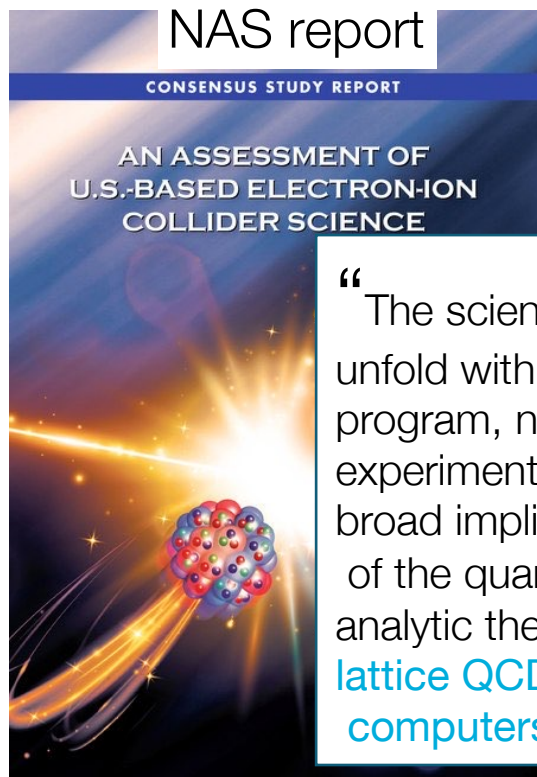
- how are partons inside the nucleon distributed in both momentum and position space?
- how do the nucleonic properties such as mass and spin emerge from partons and their underlying interactions?
- how do the confined hadronic states, including QCD Goldstone bosons, emerge from these quarks and gluons?

Lattice calculations of GPDs, TMDs and high momentum form-factors

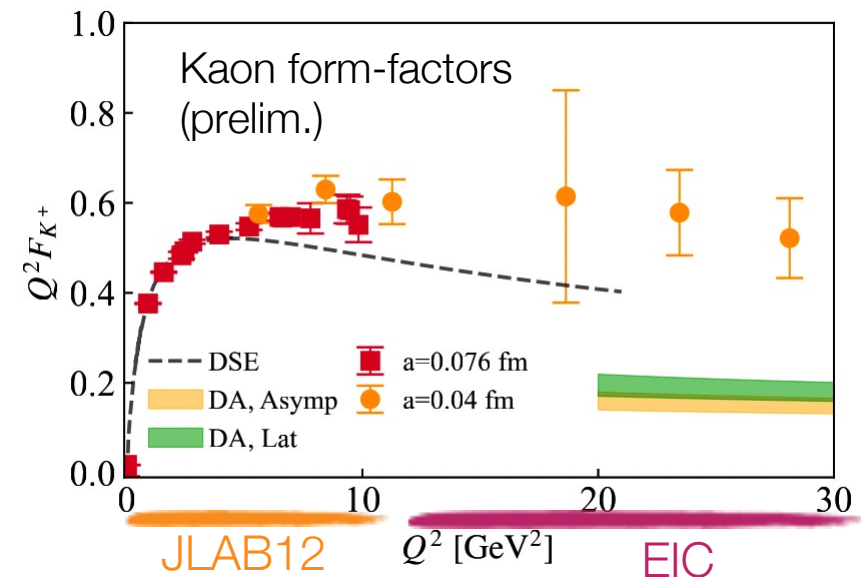
⇒ Highly boosted hadrons on the lattice

⇒ Challenges: small lattice spacing, noise problem

Algorithmic developments
Exa-scale computing resources
are needed



“The scientific challenges that would unfold with EIC require a robust theory program, not simply to design and interpret experiments, but also to develop the broad implications in an understanding of the quantum world, both through analytic theory as well as through lattice QCD simulations on large-scale computers.”



Cold QCD: hadron spectroscopy, nuclei and tests of fundamental symmetries

What is the spectrum the confined hadronic states ?

How do the quark-gluon interactions create nuclear binding?

What are the short distance properties of nuclei ?

Lattice calculations of light nuclei with unphysical quark masses:

- Magnetic moments and polarizabilities
 - Quenching of axial charge
 - Nuclear PDF, EMC effect
 - Lattice calculation of $nn \rightarrow ppee$ process (A. Grebe, Z. Fu, Lattice 2022)
- input for EFT : important for neutrinoless double beta decay
(Algorithmic progress tracking complicated contractions of two electroweak current insertions)

Hadron spectroscopy:

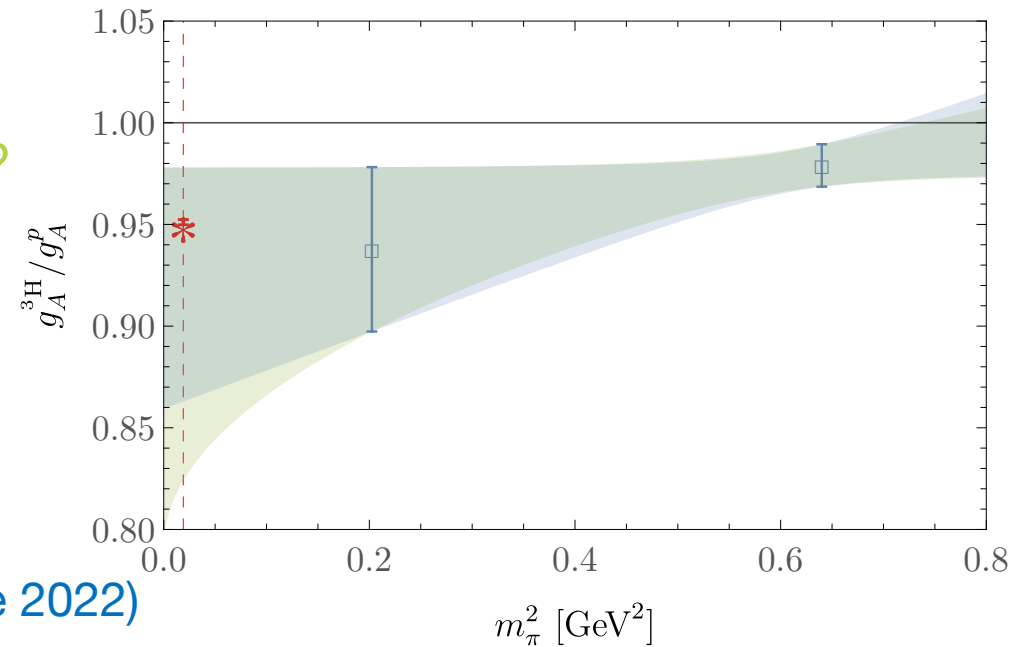
First ever study of full decay of exotic: π_1 is a broad resonance

(new search strategies for GlueX), Woss et al. (HadSpec), Phys. Rev. D 2021

New frontier: 3-particle amplitude calculations on the lattice

Blanton et al, JHEP 2021, Hansen et al. PRL 2021

Will allow to study more complex resonances, a_1 , Roper etc. Challenge: Contractions cost increase rapidly



Algorithmic developments
exa-scale computing resources
are needed to perform calculations
for physical quark mass

Exascale Computing Project (ECP)

- LQCD is a major ASCR project to develop software and applications for exascale machines at Aurora at ANL & Frontier at ORNL.
- Lattice QCD is one of the 11 applications selected to compose one of the KPPs of the project



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NEW COMPUTATIONS ON SCATTERING AMPLITUDES ILLUMINATE QUARK AND GLUON PARTICLE INTERACTIONS

July 6, 2021

A transatlantic team of researchers has provided the first calculation of the full relativistic scattering amplitude for a three-hadron system of particles, which lies at the core of outstanding questions in quantum chromodynamics. The analytical and computational methods developed in this work pave the way for future calculations in more complicated systems involving multiparticle and nuclear systems. The researchers' findings, which support the GlueX experiment at Thomas Jefferson National Accelerator Laboratory and other programs around the world, were published in the January 2021 issue of *Physical Review Letters* as an Editor's Suggestion.

The majority of visible matter in the universe is composed of quarks and gluons. Experiments at particle and nuclear physics labs around world investigate the mass, spin, and structure of single hadrons—particles composed of quarks and gluons—as well as multihadron systems using scattering amplitudes to reconstruct and discern the internal structure of hadrons. The determination of scattering amplitudes involving two particles is fairly well established, but challenges remain for three-particle systems. The team's work addresses challenges associated with constructing amplitudes that obey fundamental properties and symmetries consistent with relativity and quantum mechanics.

Recently in *Physical Review D*, the team presented the first computation of the decays of an exotic meson, a state in which the gluon degrees of freedom are manifest. This additional research predicts the existence of such a state and provides the rates for decay particle pairs. Future calculations will probe the internal structure of states of quarks and gluons through the computation of matrix

Computational Nuclear Physics and AI/ML Workshop

Priorities for the next decade

We recommend investments in computational nuclear physics to accelerate discoveries and maintain U.S. leadership by:

- Strengthening programs and partnerships to ensure the efficient utilization of new HPC hardware and new capabilities and approaches offered by AI/ML and quantum computing (QC);
- Establishing programs that support the education and training of a diverse and multidisciplinary workforce with cross-disciplinary collaborations in HPC, AI/ML, and QC;
- Expanding access to dedicated hardware and resources for HPC and new emerging computational technologies.

<https://indico.jlab.org/event/581/timetable/>