

Fundamental nuclear physics at the exascale and beyond

**Robert Edwards
Jefferson Lab**

Fundamental nuclear physics at the exascale

LQCD ASCR/NP SciDAC-5

- Argonne:
 - Robert Latham
 - Robert Ross → Sandeep Madireddy
 - Yong Zhao
- Brookhaven:
 - Swagato Mukherjee
- JLab
 - Jie Chen
 - Robert Edwards
 - Eloy Romero
 - Frank Winter
- Lawrence Berkeley
 - Aydin Buluc
 - Sherry Li
 - Andre Walker-Loud
- Los Alamos
 - Tanmoy Bhattacharya
- MIT:
 - Saman Amarasinghe
 - Will Detmold
 - Andrew Pochinsky
 - Phiala Shanahan
- Oak Ridge:
 - Prasanna Balaprakash
 - Henry Monge Camacho
- William & Mary:
 - Kostas Orginos
 - Andreas Stathopoulos
- NVIDIA:
 - Kate Clark
 - Balint Joo

Publicity and useful repositories

Website: <https://lqcdscidac.github.io>



ASCR/NP LQCD SciDAC Project

[Home](#) [About](#) [SciDAC](#) [Highlights](#) [People](#) [Publications](#)

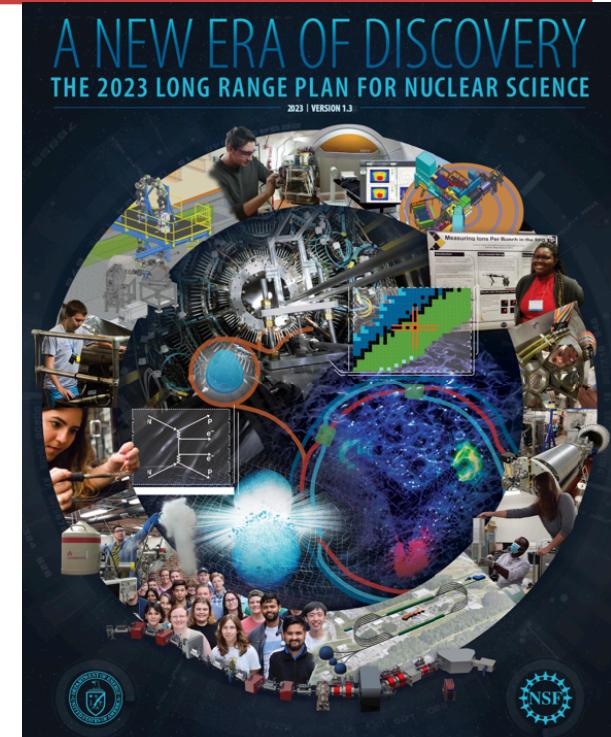
ASCR/NP LQCD SciDAC Project

The Lattice Quantum Chromo-Dynamics (LQCD) ASCR/NP SciDAC Project is supported by the U.S. Dept. of Energy Office of Nuclear Physics and the Office of Advanced Scientific Computing Research. This SciDAC project focuses on an ambitious program of theoretical, algorithmic and software development which will enable calculations using lattice Quantum Chromodynamics (LQCD) methods to exploit the new generation of leadership-class resources and dedicated hardware to address fundamental questions in nuclear science. Specifically, our project will impact our understanding of results from current heavy ion experiments at the Relativistic Heavy-Ion Collider (RHIC), the study of excited and exotic states of hadrons at CLAS-12 and GlueX at Jefferson Lab (JLab) and the hadron and nuclear structure programs at RHIC-spin and JLab. The calculations that are enabled by the proposed developments will also look forward to experiments on protons and nuclei at the upcoming Electron-Ion Collider (EIC).

Scientific goals of project

Science areas recognized in the 2023 NSAC Long Range Plan

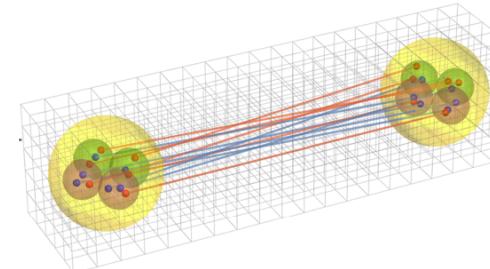
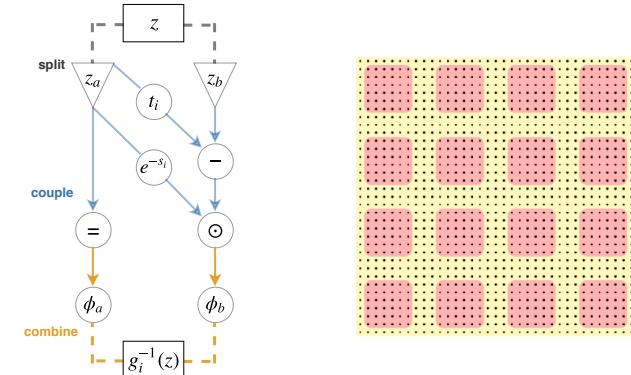
- Hadron spectroscopy
 - *Determine spectrum and internal structure of QCD exotic states*
 - Impact CLAS12 & GlueX @ JLab, and possible CEBAF upgrade
- Hadron structure
 - *Build 3D image of proton in its entirety*
 - JLab 12 & future EIC @ BNL
- Partonic structure of nuclei
 - *Improve constraints on distribution functions of nuclei though A=7*
 - Future EIC, future DUNE (FNAL) & HyperK (Japan)
- Extreme matter - quark gluon plasma
 - *Characterize quark gluon plasma via spectrum of heavy quarks*
 - sPHENIX @ BNL and LHC @ CERN



SciDAC-5 partnership - ASCR & NP

Three main themes:

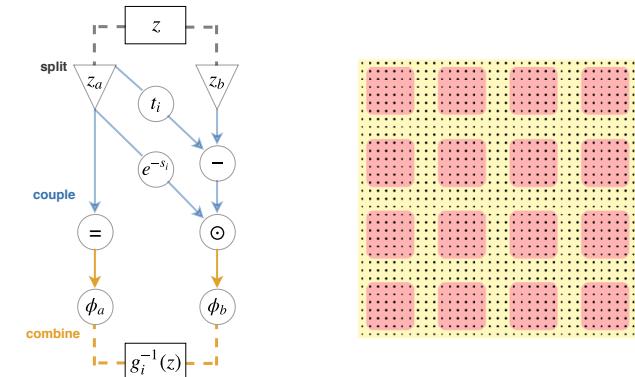
- Gauge-field generation
 - *Use ML and hierarchically structured sampling*
 - Impact - radically increase fidelity and statistics of calculations
- Analysis
 - *Linear system solvers and many-body correlation function computations*
 - Impact - extract ever more sophisticated physics processes
- Changing computational landscape
 - *Code-portability and development for new hardware architectures*
 - Impact - utilize advanced capabilities of Frontier, Aurora, NERSC-10 & OLCF-6



SciDAC-5 partnership - ASCR & NP

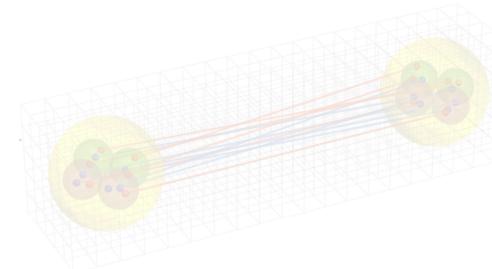
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See talk by Yixuan Sun & Eloy Romero & Sherry Li

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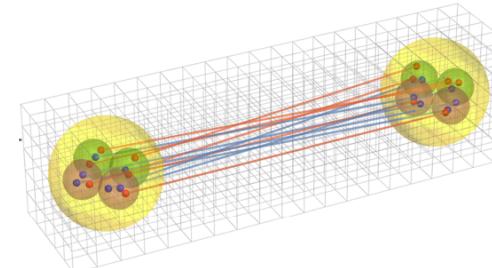
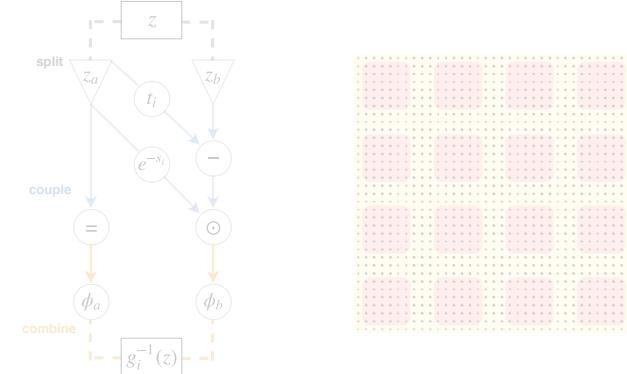
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See talk Eloy Romero & Sherry Li & Aydin Buluc

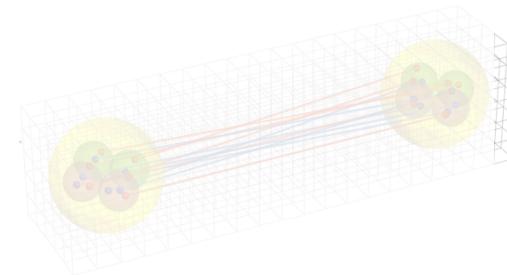
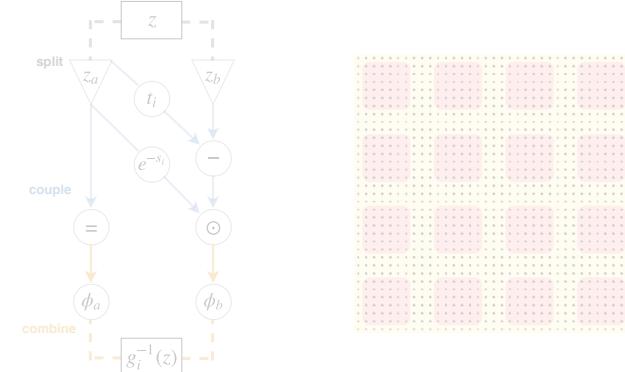
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Collaboration with ASCR

Workforce

GS, PD-s, junior staff supported/trained

Person	Position	Institution
Ryan Abbott	Graduate Student (NP)	MIT
Willow Ahrens	Graduate Student (ASCR)	MIT
Dennis Bollweg	Postdoctoral Researcher (NP)	BNL
Noah Chavez	Undergraduate Student (NP)	BNL
Sam Christian	Undergraduate Student (NP)	MIT
Teodoro Collin	Graduate Student (ASCR)	MIT
Herve Dutrieux	Postdoctoral Fellow (NP)	W&M
Srinivas Eswar	Postdoctoral Scholar (ASCR)	ANL
Jinchen He	Graduate Student (ANL)	BNL
Xiang Gao	Postdoctoral Researcher (NP)	BNL
Joshua Lin	Graduate Student (NP)	MIT
Emin Ozturk	Graduate Student (ASCR)	LBNL
Oguz Selvitopi	Junior Staff (ASCR)	LBNL
Qi Shi	Graduate Student (NP)	BNL
Hai-Tao Shu	Postdoctoral Researcher (NP)	BNL
Ben Slimmer	Graduate Student (NP)	W&M
Richard Sollee	Undergraduate/MEng Student (ASCR)	MIT
Yixuan Sun	Postdoctoral Scholar (ASCR)	ANL
Fei Yao	Postdoctoral Researcher (NP)	BNL

Awards

Recognitions of achievement including career advancement

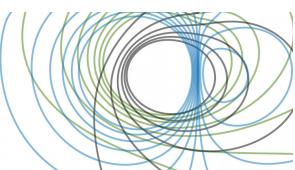
Person	Position	Institution	Award	Body
Ryan Abbott	Grad. Student	MIT	DOE HEP Comp. Traineeship	HEP
Dennis Bollweg	Postdoc	BNL	Staff Hire (Asst. Sci.)	BNL
Sam Christian	Grad. Student	MIT	Hertz Foundation Finalist	Hertz
William Detmold	Faculty	MIT	Elected USQCD Deputy Chair	USQCD
Gurtej Kanwar	Postdoc	MIT	Faculty Hire	U. Edinburgh
Swagato Mukherjee	Staff	BNL	BNL Sci. & Tech. Award	BNL
Phiala Shanahan	Assoc. Prof.	MIT	Ruby Payne-Scott Award	Aust. Inst of Physics
Phiala Shanahan	Assoc. Prof.	MIT	Tenured	MIT
Hai-Tao Shu	Postdoc	BNL	Asst. Prof.	Central China Normal U.
Ben Slimmer	Grad. Student	W&M	DOE-SCGSR	DOE
Michael Wagman	Staff	MIT	Ken Wilson Award	Lattice Conf. Series
Yong Zhao	Staff	ANL	Ken Wilson Award	Lattice Conf. Series
Yong Zhao	Staff	ANL	Guido Altarelli Award	Int. Spin Phys.

Some highlights



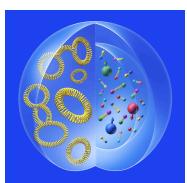
Drilling into Neutron Stars with Computers

Simulations of neutron stars provide new bounds on their properties, such as their internal pressure and their maximum mass.



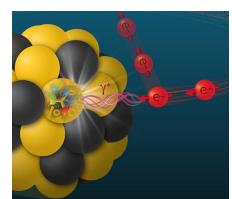
Inside the box - look at excited hadrons could help solve mystery of particle X3872

Lattice QCD method suggests a simpler spectrum of exotic XYZ hadrons



Gravitational Form Factors Illuminate Substructure of the Proton

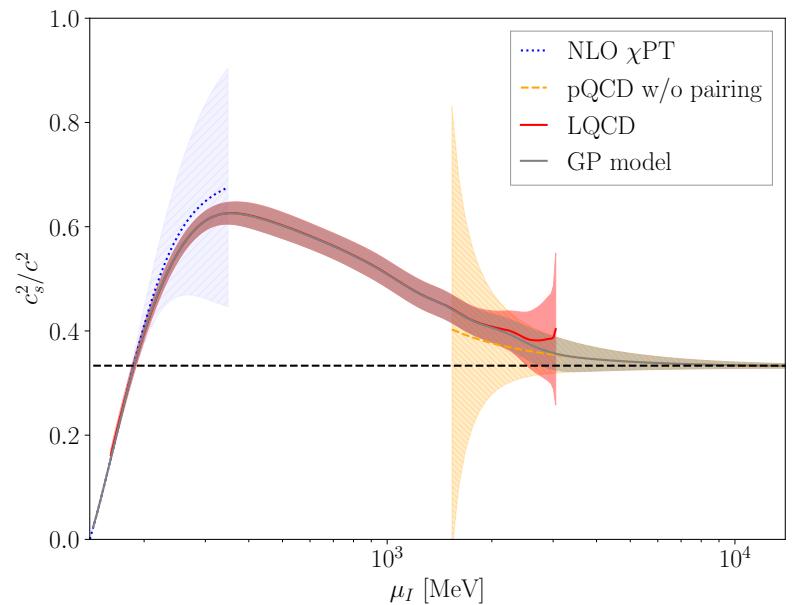
LQCD to understand for the first time certain aspects of proton structure in terms of its fundamental quark and gluon constituents



Scientists Calculate Predictions for Electron-Ion Collider Measurements

Calculations of charge distribution in mesons provide a benchmark for experimental measurements and validate widely used 'factorization' method.

Drilling into Neutron Stars with Computers



[Phys. Rev. Lett. 134:011903, Jan 2025](#)

APS Viewpoint:
[*Drilling into Neutron Stars with Computers*](#)



Simulations of neutron stars provide new bounds on their properties, such as their internal pressure and their maximum mass.

Accomplishment: Determination of equation-of-state (EoS) for isospin-dense matter and constraints on EoS for symmetric nuclear matter.

Methods: Many pion contractions and code optimizations developed under SciDAC.

Impact: Speed of sound greater than conformal bound. Implies neutron stars can grow > 2 solar masses

- Talks

- Eloy Romero (JLab)
- Sherry Li (LBNL)
- Yixuan Sun (ANL)
- Aydin Buluc (LBNL)

Workshop report:

Software Infrastructure for Advanced
NP Computing: [arXiv:2501.00905](https://arxiv.org/abs/2501.00905)

- Posters

- Improving Preconditioners for LQCD - Eloy Romero
- Gauge field generation with Exponentiated Clover Fermions - Henry Comacho
- Graphs and tensor contractions - Eloy Romero
- Exploring gauge-fixing conditions with gradient-based optimization - Will Detmold

SciDAC Goals - Gauge field generation with ML

Simulations: lattice gauge fields the building block for all LQCD science campaigns

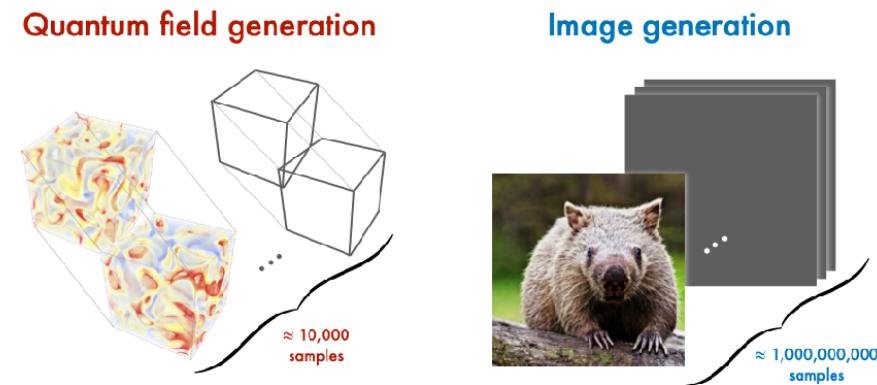
Importance: Future spectroscopy and structure projects need increased fidelity - smaller lattice spacings and much larger statistics

Challenge: Generation suffers from critical-slowing down
Higher fidelity → vastly increased computing requirements

Science goal: (killer app): Holy Grail of LQCD

Approach:

- Partnership with **RAPIDS & FastMath**
- Machine-learning for gauge generation & preconditioners



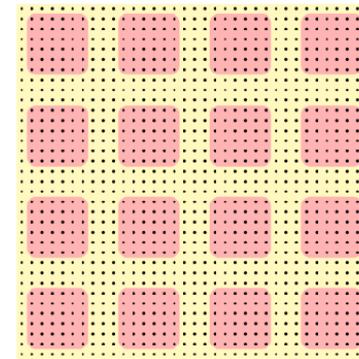
K. Cranmer (incl. P. Shanahan), Nature Rev. Phys. 5 (2023) 9, 526-535

See talk by Yixuan Sun

SciDAC Goals - Hierarchical gauge generation & integration

Simulations: combine gauge generation and measurements

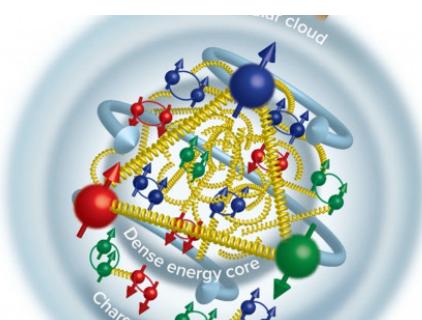
Disconnected subdomains (red) - buffers (yellow)



Importance: radically increase statistics

Challenge: divide the lattice into subdomains & integrate independently. Careful control of determinant

Science goal: (killer app): High statistics computation of gluonic observables within hadron structure



Approach:

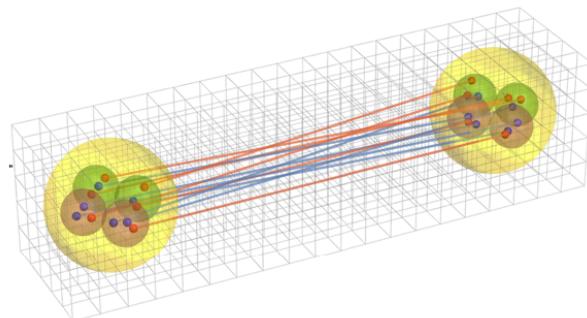
- Partnership with **FastMath**

Bride, Giusti, Harris, Pepe, Phys. Lett. B 816, 136191 (2021)

See talk by Eloy Romero & Sherry Li

SciDAC Goals - Analysis

Simulations: computing Euclidean correlation functions



Importance: bread & butter of LQCD. Enable more sophisticated measurements

Challenge: many-body contractions generate large temporaries

Science goal: (killer app): Multi-meson+baryon systems including nuclei

Approach:

- Partnership with **RAPIDS**

See talk by Eloy Romero & Aydin Buloc

Products under this SciDAC-5

Total of 72 products + 4 DOE SC highlights + 11 news articles

Several news articles in pipeline for DOE highlights

Full listing of all letters, articles, proceedings, preprints and codes in report

Product summary	
Type	Number
DOE Highlights	(4)
News articles	(11)
Letters	9
Articles	28
Proceedings	15
Pre-prints	8
Cites \geq 50	(5)
Theses	1
Code repositories	11
Total	72

SciDAC Goals - Changing computational landscape

Simulations: increase portability of software

Importance: efficiently utilize next generation systems

Challenge: requires investment in code-portability for each new system

Approach:

- Partnership with **RAPIDS & FastMath**

See talks by Aydin Buluc & Sherry Li

Workshop report:

Software Infrastructure for Advanced
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SciDAC-5 is a partnership

- Strong partnerships with **FastMath & Rapids**, and ASCR/NP supported community
- SciDAC a huge boost for LQCD & NP
 - present science was not possible 10 years ago
 - fresh perspective on entire program
- Is significantly impacting our calculations
 - huge advance in gauge generation - accelerated our science campaigns
 - accelerating analysis campaigns on leadership & local resources
 - better tools for (more easily) improving performance

