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

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

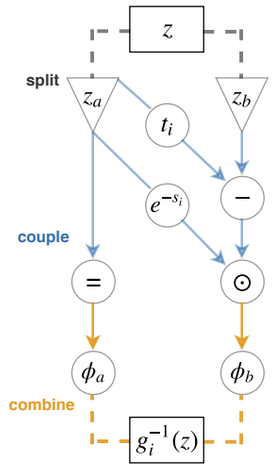
- Hadron structure
  - *Build 3D image of proton in its entirety*
  - JLab 12 & future EIC @ BNL

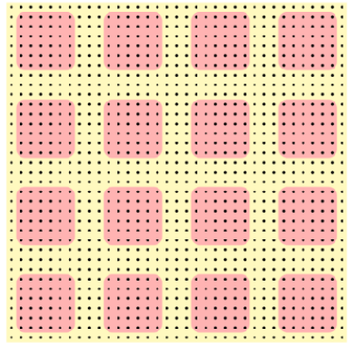
- Partonic structure of nuclei
  - *Improve constraints on distribution functions of nuclei though A=7*
  - Future EIC, future DUNE (FNAL) & HyperK (Japan)

- Extreme matter - quark gluon plasma
  - *Characterize quark gluon plasma via spectrum of heavy quarks*
  - sPHENIX @ BNL and LHC @ CERN

SciDAC-5 partnership - ASCR & NP

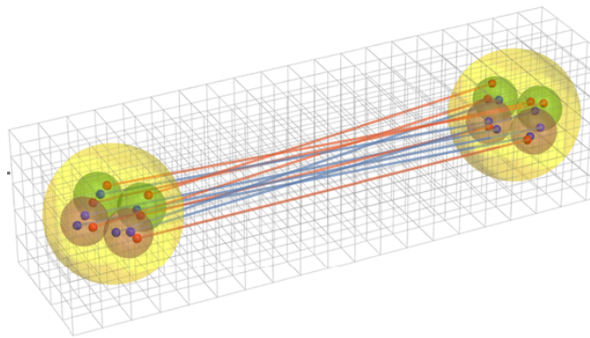
Three main themes:





- 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

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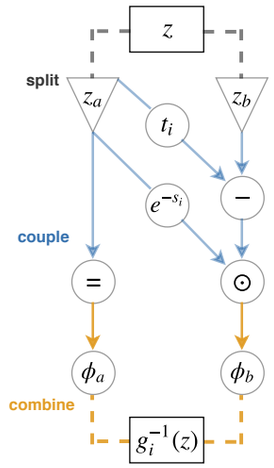

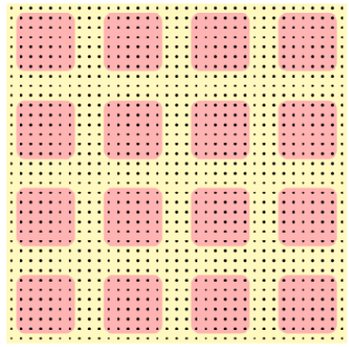

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See talk by Yixuan Sun & Eloy Romero & Sherry Li

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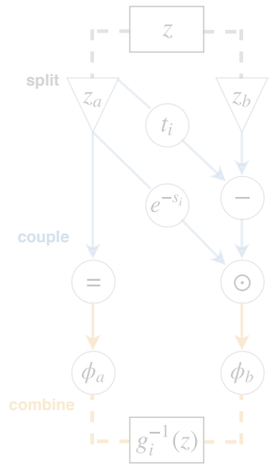

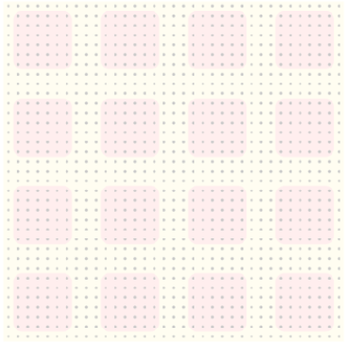

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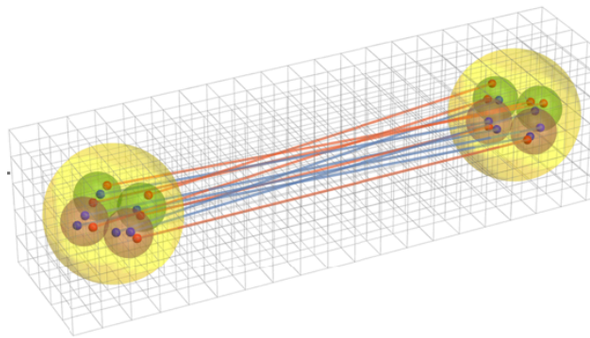

See talk Eloy Romero & Sherry Li & Aydin Buluc

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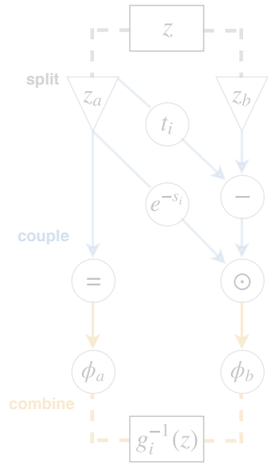

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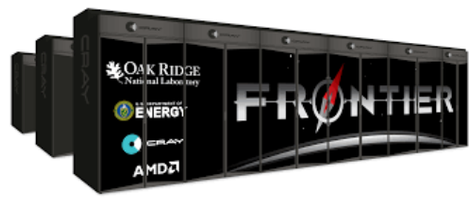


Collaboration with ASCR

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

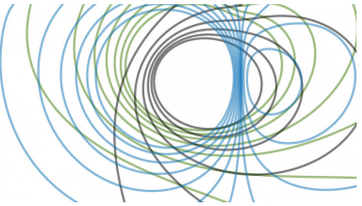
Recognitions of achievement including career advancement

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

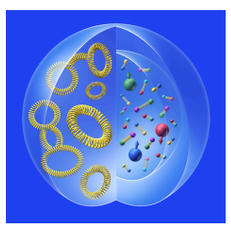
Drilling into Neutron Stars with Computers

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



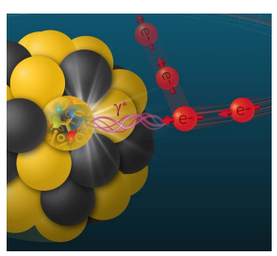
Inside the box - look at excited hadrons could help solve mystery of particle X3872

Lattice QCD method suggests a simpler spectrum of exotic XYZ hadrons



Gravitational Form Factors Illuminate Substructure of the Proton

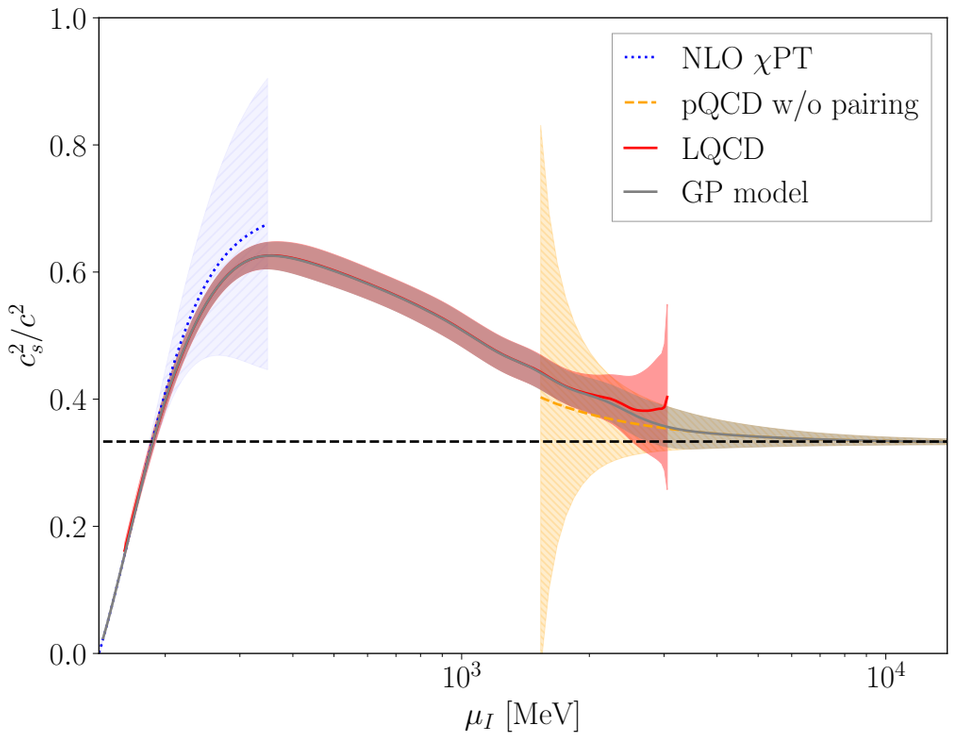
LQCD to understand for the first time certain aspects of proton structure in terms of its fundamental quark and gluon constituents



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 & posters today

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

Workshop report:

Software Infrastructure for Advanced NP Computing: arXiv: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

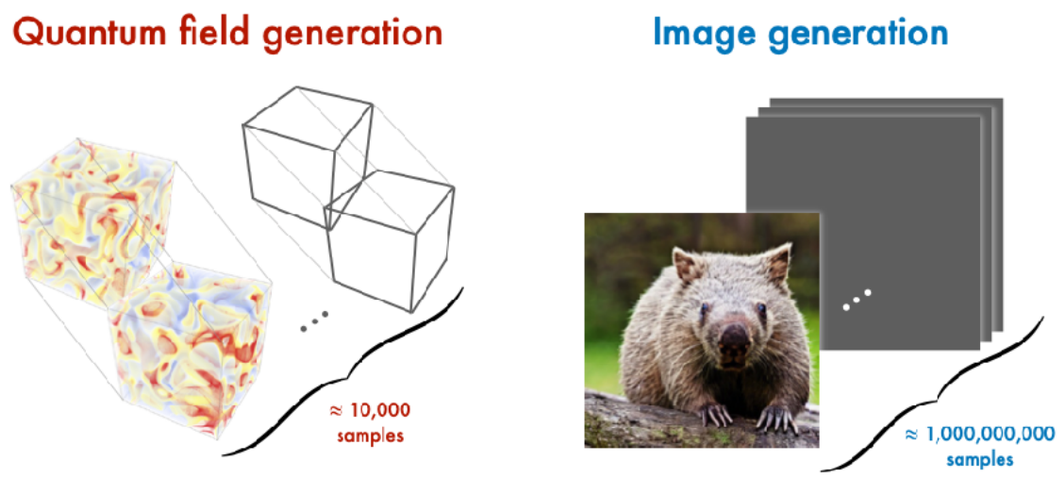
SciDAC Goals - Gauge field generation with ML

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



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

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

Approach:

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

See talk by Yixuan Sun

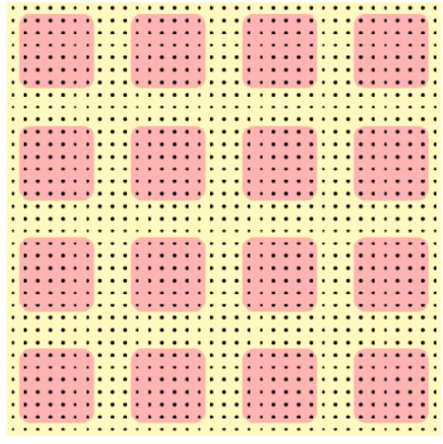
SciDAC Goals - Hierarchical gauge generation & integration

Simulations: combine gauge generation and measurements

Importance: radically increase statistics

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

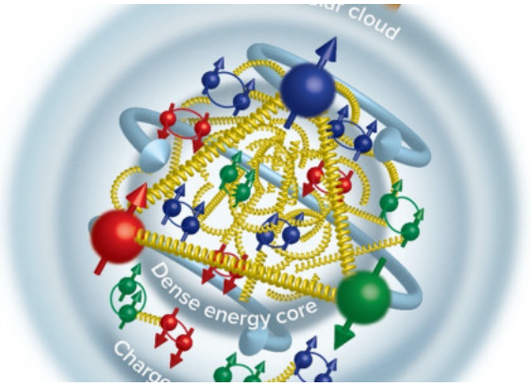
Disconnected subdomains (red) - buffers (yellow)



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

Approach:

- Partnership with FastMath

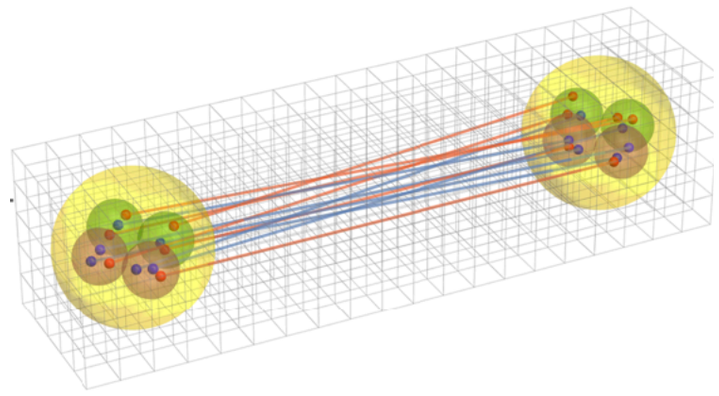


Bride, Giusti, Harris, Pepe, Phys. Lett. B 816, 136191 (2021)

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

Product summary

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

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

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 NP Computing: arXiv:2501.00905

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