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
  - Yong Zhao
- Brookhaven:
  - Swagato Mukherjee
- JLab
  - Jie Chen
  - Robert Edwards
  - Eloy Romero
  - Frank Winter
- Lawrence Berkeley
  - Aydin Buluc (& Oguz Selvitopi)
  - Sherry Li
  - Andre Walker-Loud
- Los Alamos
  - Tanmoy Bhattacharya (& Jun-Sik Yo)
- 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

GitHub: https://github.com/LQCDSciDAC   Website: https://lqcdscida.github.io

SciDAC
Scientific Discovery through Advanced Computing

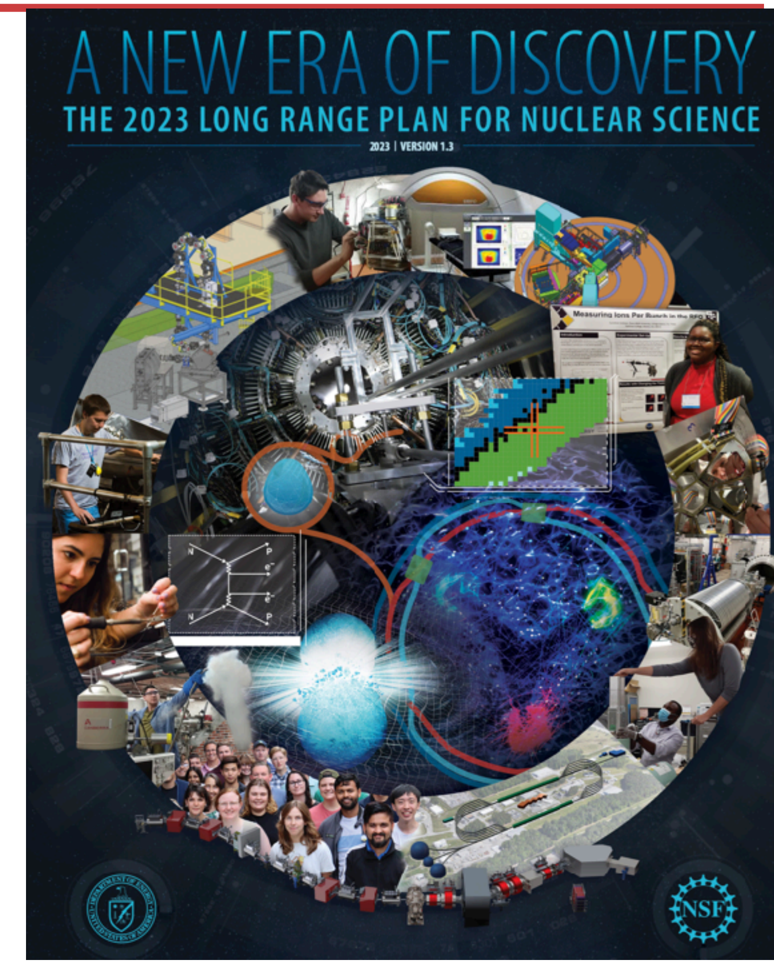
ASCR/NP LQCD SciDAC Project

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

ASCR/NP LQCD SciDAC - fundamental NP at Exascale

ASCR/NP LQCD SciDAC

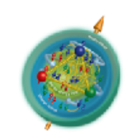
- **Hadron Spectrum:**

$\mathcal{L}_{\mathrm{QCD}}$ → Lattice QCD →

Resonances & exotic/hybrid hadrons

- **Hadron Structure:**

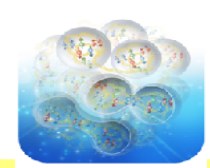
$\mathcal{L}_{\mathrm{QCD}}$ → Lattice QCD →



Hadron 3D imaging

- **Nuclear Structure:**

$\mathcal{L}_{\mathrm{QCD}}$ → Low energy EFTs →

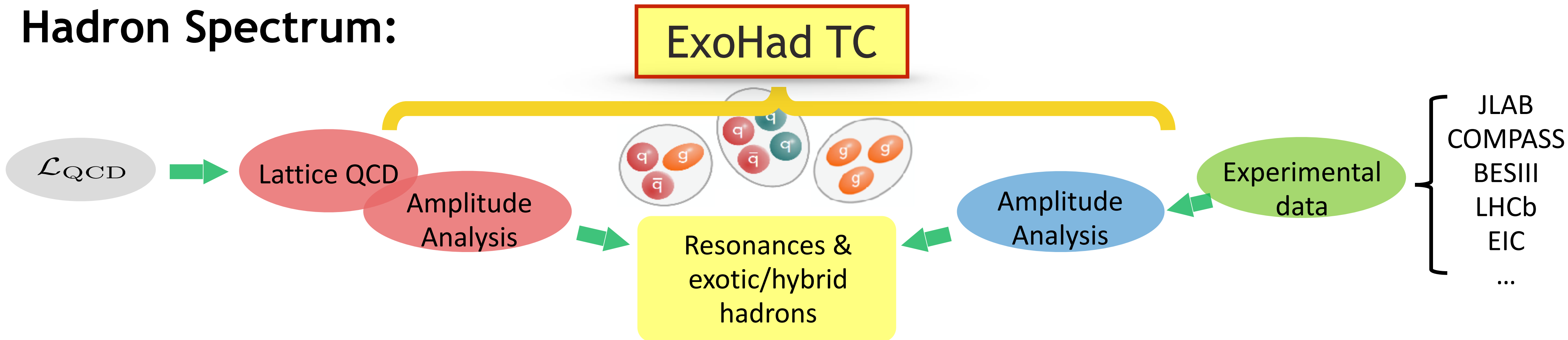


Nuclear Properties & Structure

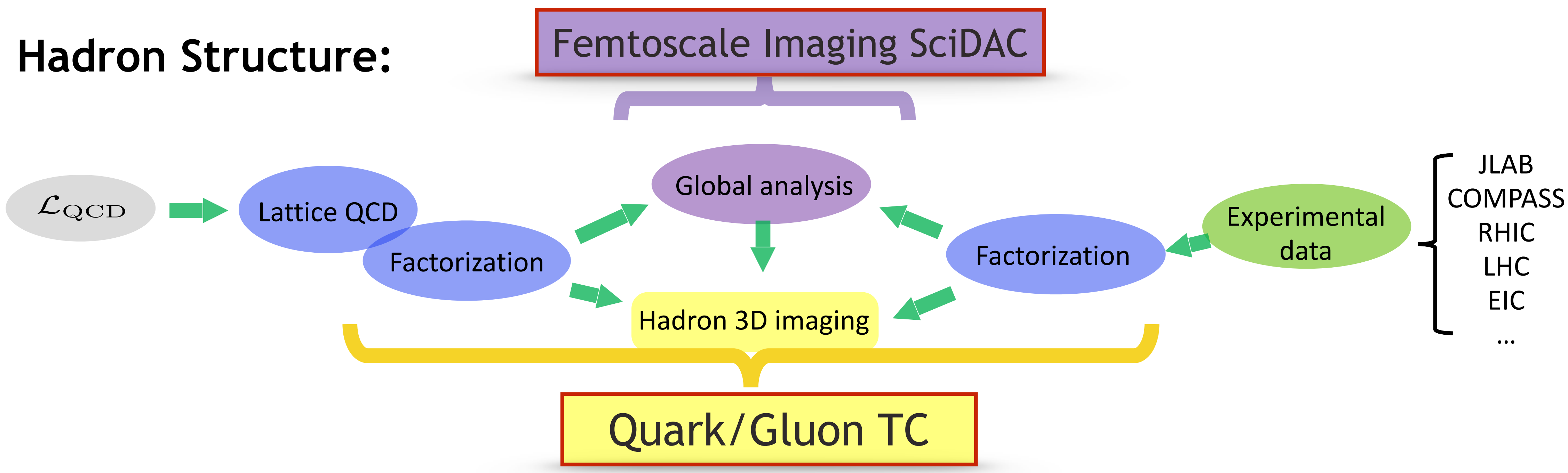
Synergy - SciDAC, Topical Collabs, & other NP projects

ASCR/NP LQCD SciDAC

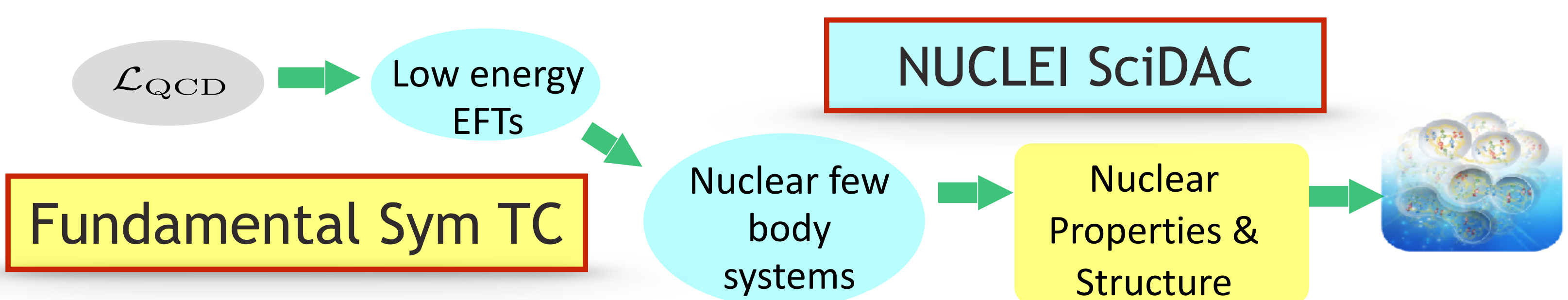
- **Hadron Spectrum:**



- **Hadron Structure:**

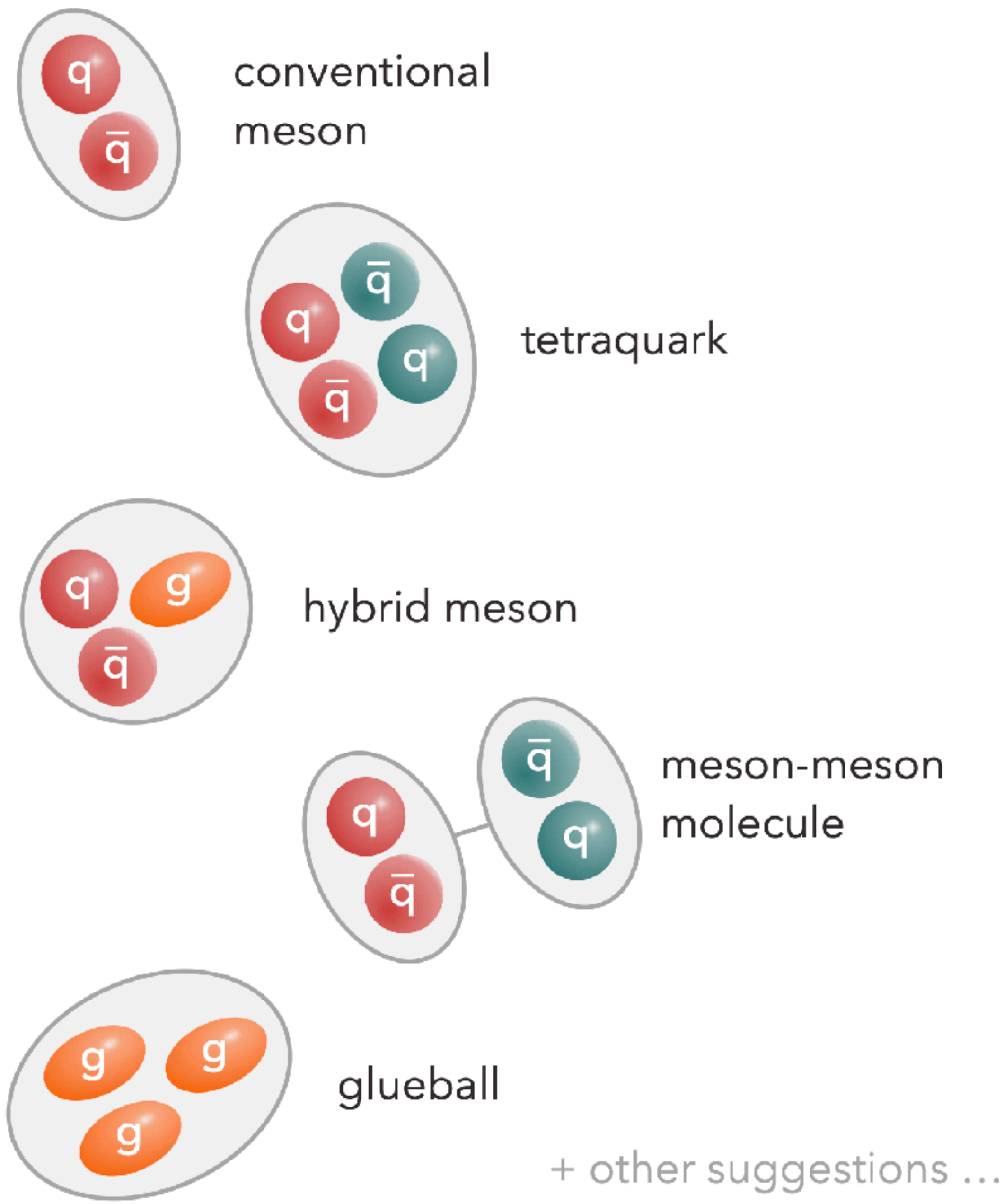


- **Nuclear Structure:**



Meson Spectroscopy

"pictures"



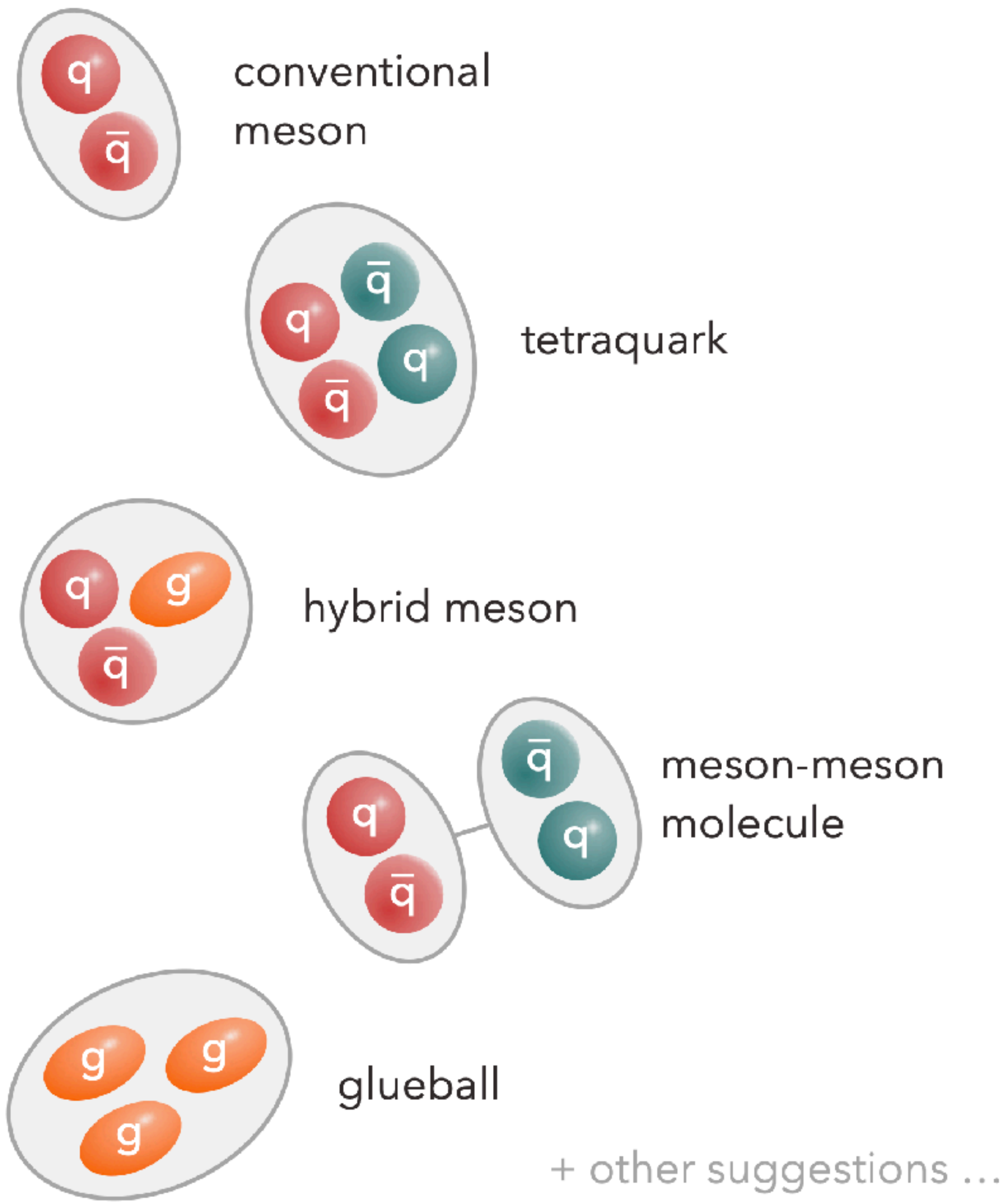
realm of modeling

connection to QCD unclear

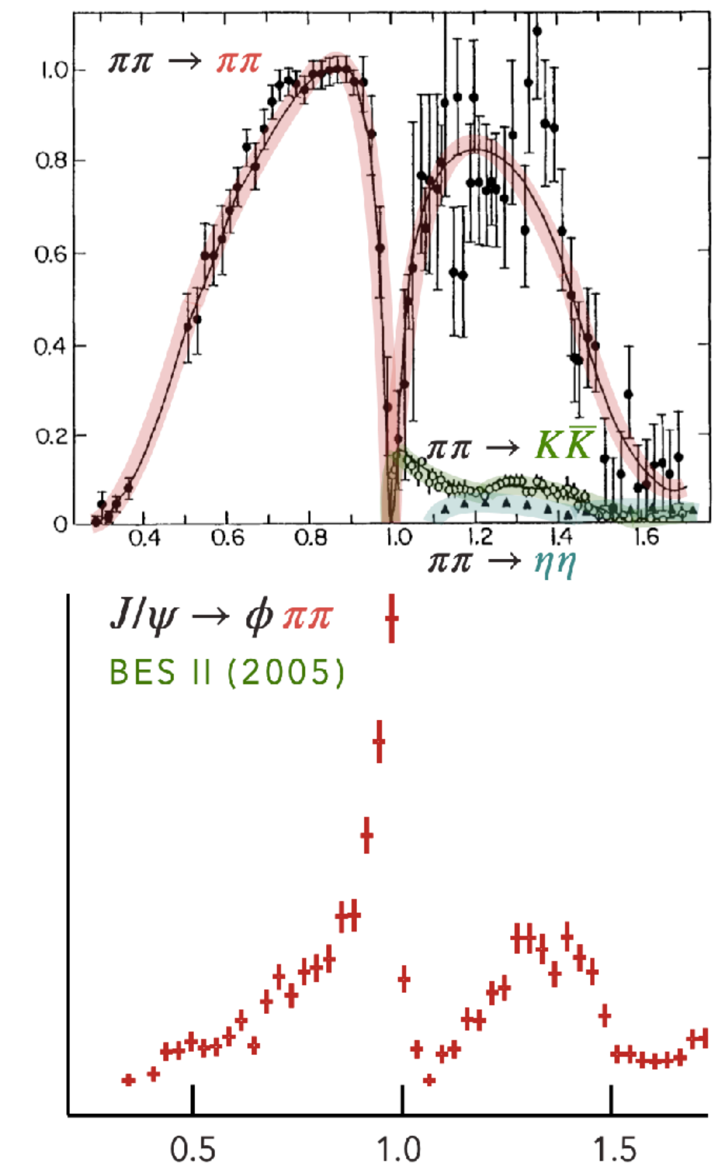
Meson Spectroscopy

“pictures”

“reality”



e.g. $f_0(980)$



realm of modeling

connection to QCD unclear

measurements of stable hadrons

connection to QCD unclear

Meson Spectroscopy

"pictures"

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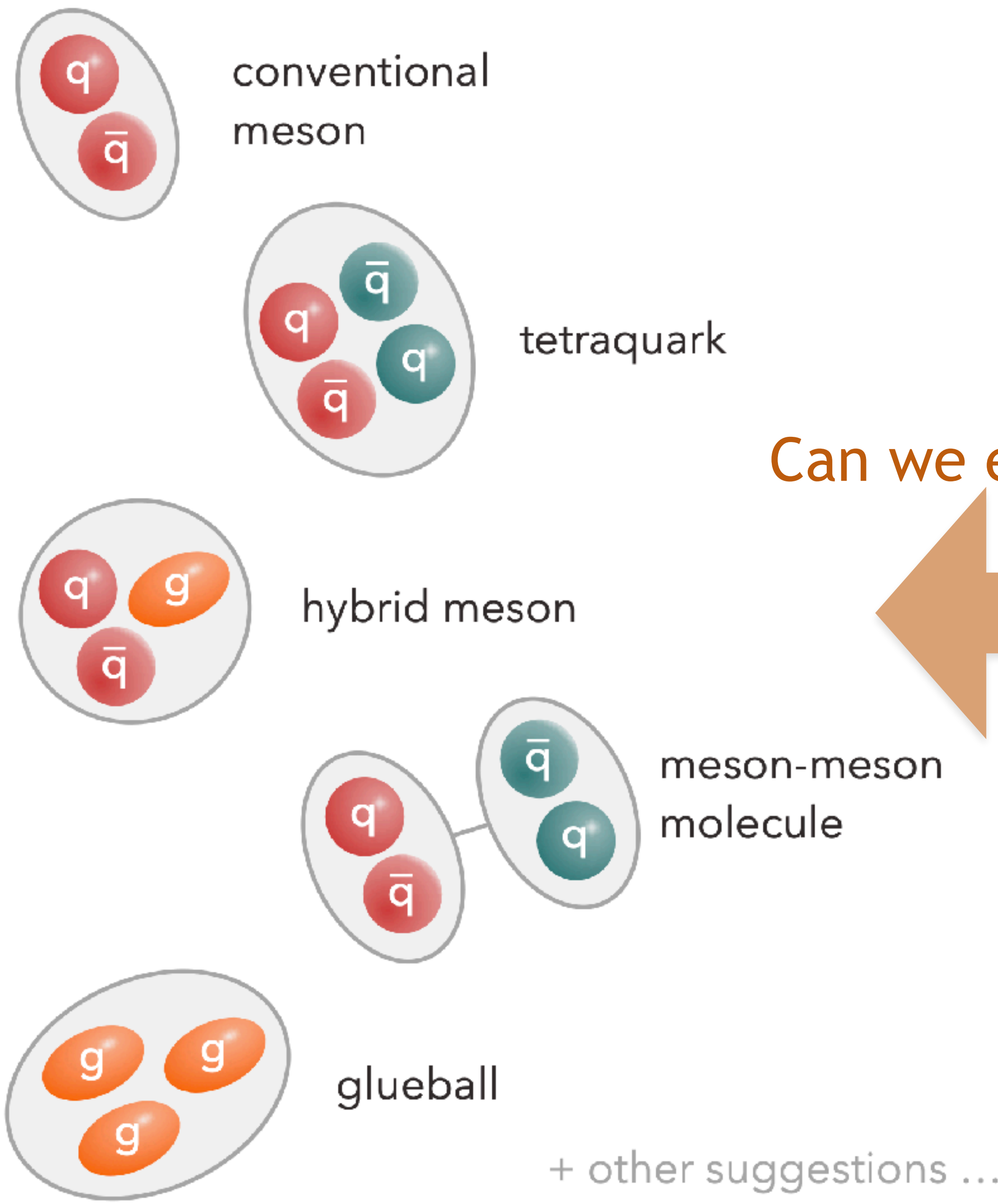
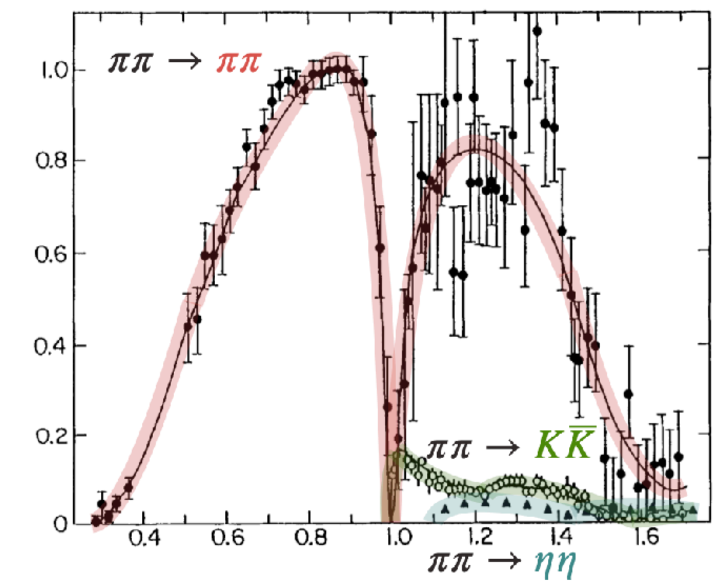
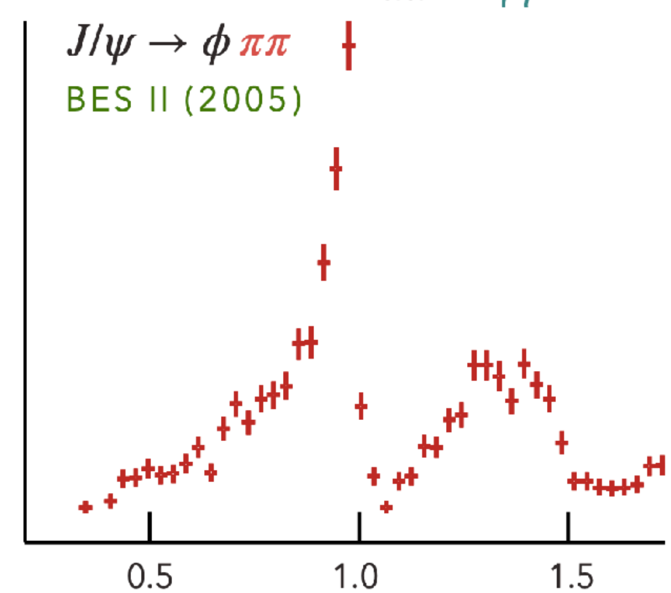


Can we establish connection?

e.g. $f_0(980)$





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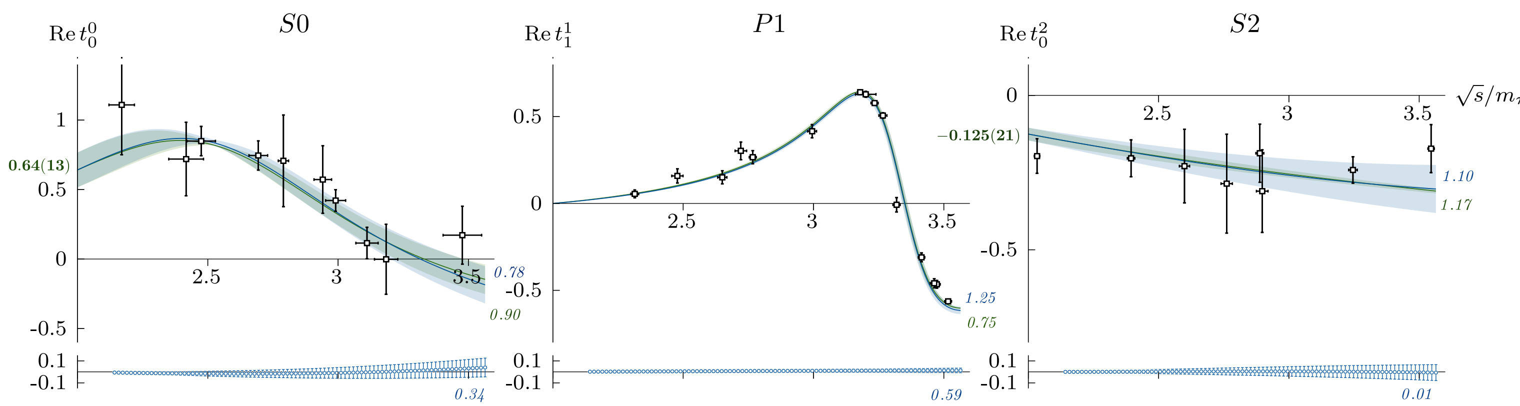
Lightest resonance of QCD

S, P, D - wave $\pi\pi$ partial waves



Quark mass dependence of lightest resonance of QCD

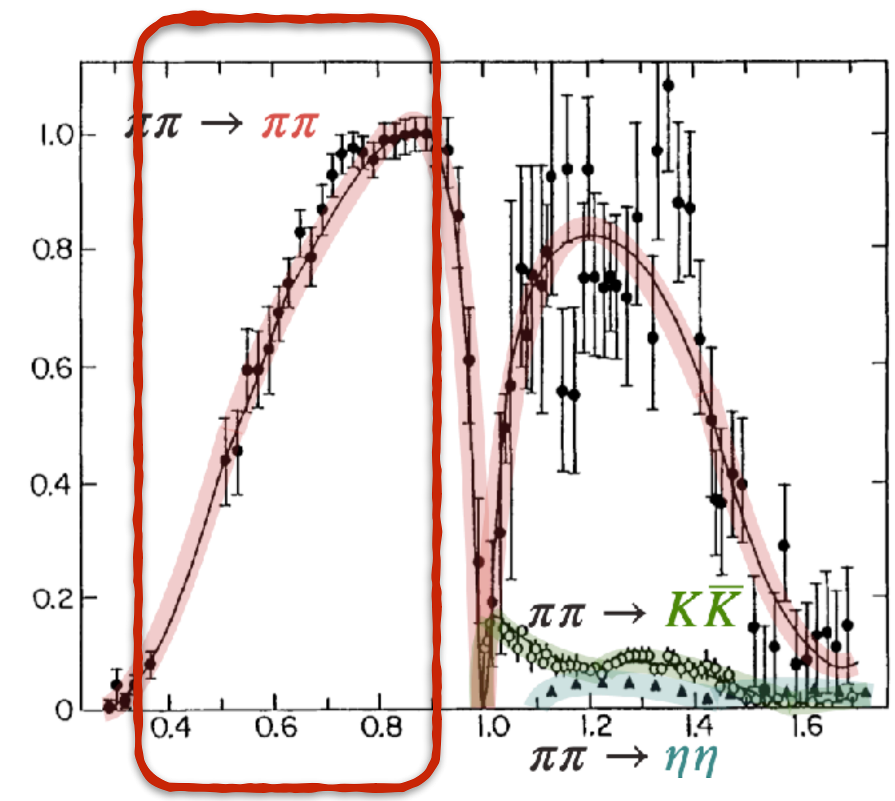
Phys.Rev. D 109 (2024) 3,3

Phys.Rev. D 108 (2023) 3,3

Accomplishment: First full QCD/characterization lightest resonance amongst quarks and gluons - 0^{++}

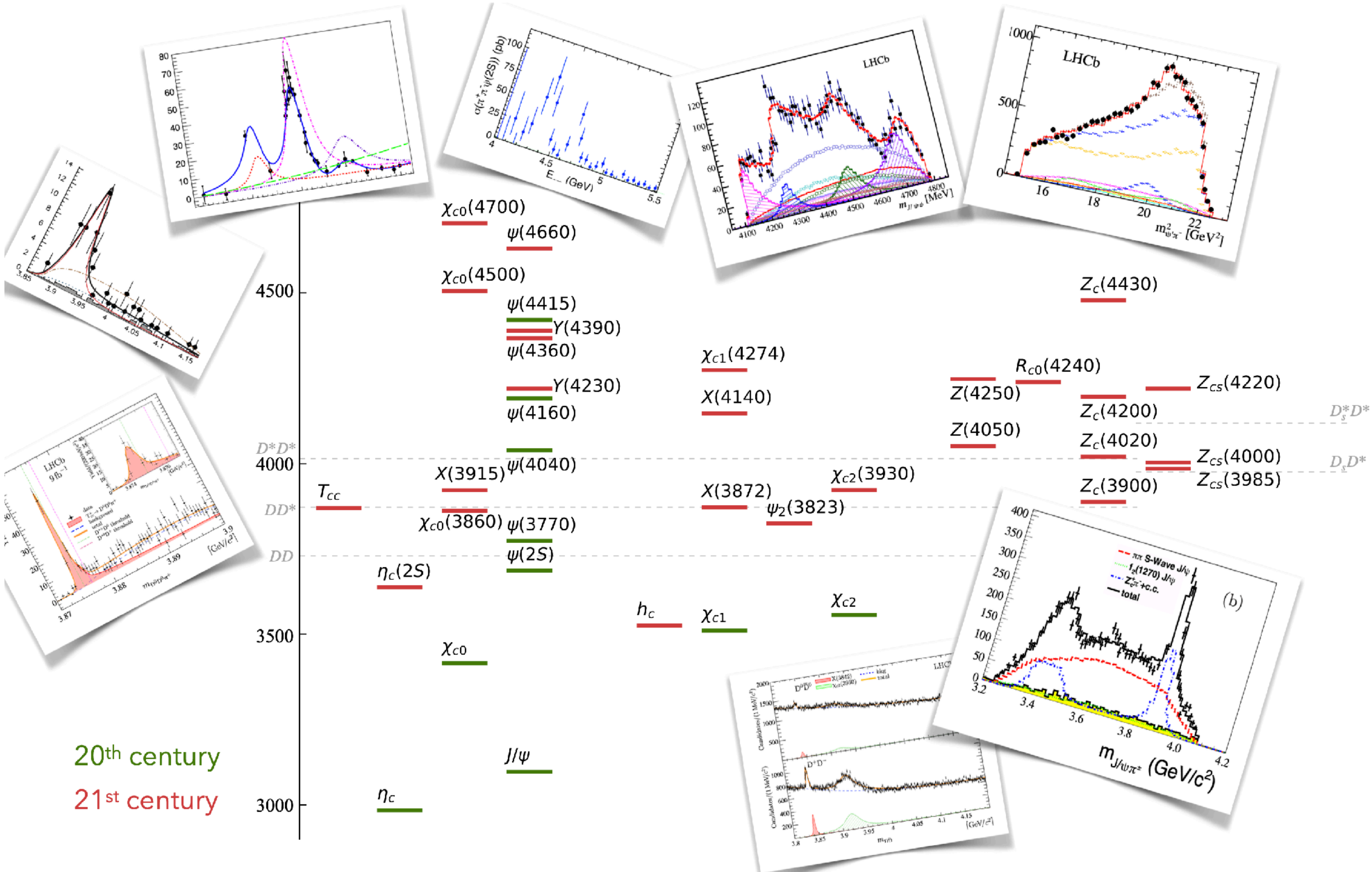
Methods: Dispersion theory essential and graph evaluation techniques essential – involving phenomenologists & RAPIDS.

Impact: Analytical/computational methods guiding the analysis campaign of the future K-long experiment @ JLab12.

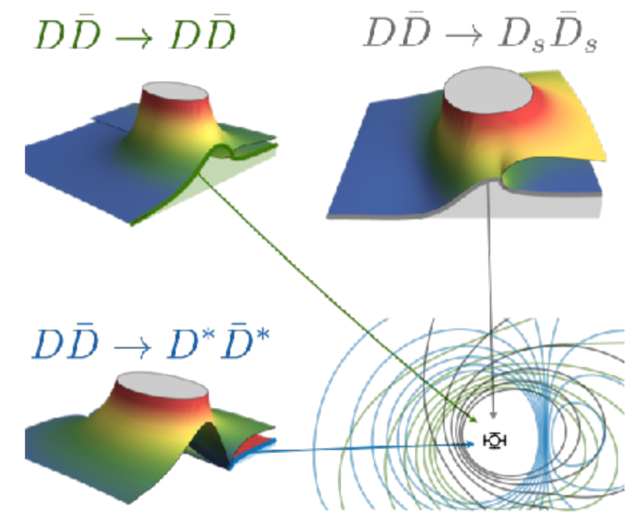


Slow rise in amplitude - resonance has weak effect in s-channel

Renewed motivation - the XYZ explosion - tetraquarks?



Charmonium resonances



Scalar and tensor charmonium resonances in coupled-channel scattering from lattice QCD

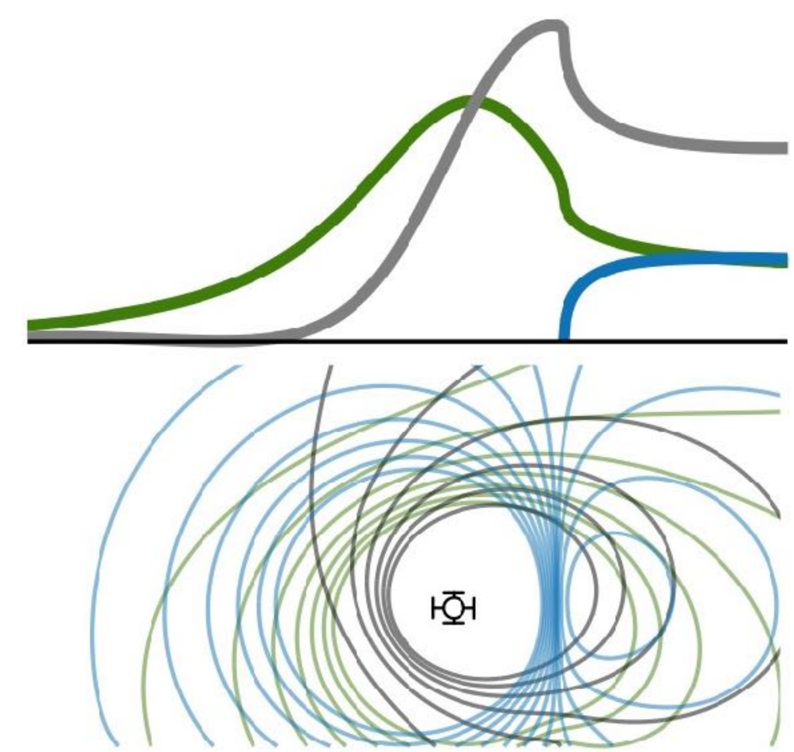
Editor's Suggestion

Phys.Rev.Lett. 132, 241901 (2024)

Phys.Rev.D 109 (2024) 11, 114503

Turning into a DOE highlight

Accomplishment:
First time: all scattering channels included in charmonium spectrum calculation



Methods: Graph evaluation techniques developed in partnership with SciDAC RAPIDS

Impact: Mapping charmonium spectrum intense focus in expts. in US, Japan, China, CERN.

Results suggests other particle production methods essential to resolve expt. picture

Charmonium resonances

Scalar and tensor charmonium resonances in coupled-channel scattering from lattice QCD

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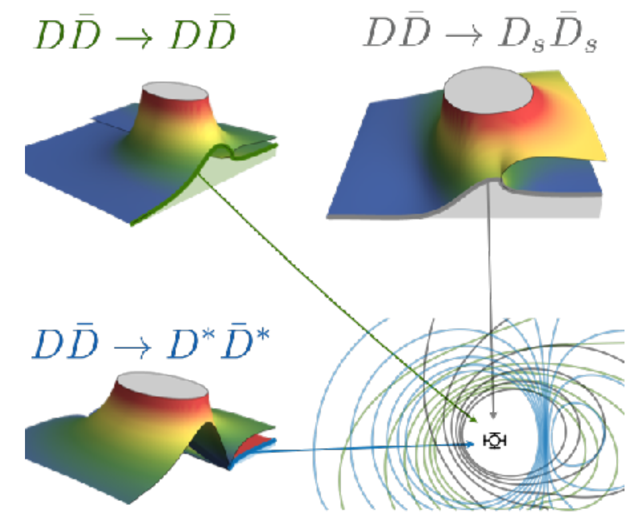


Accomplishment:
First time: all scattering channels included in charmonium spectrum calculation

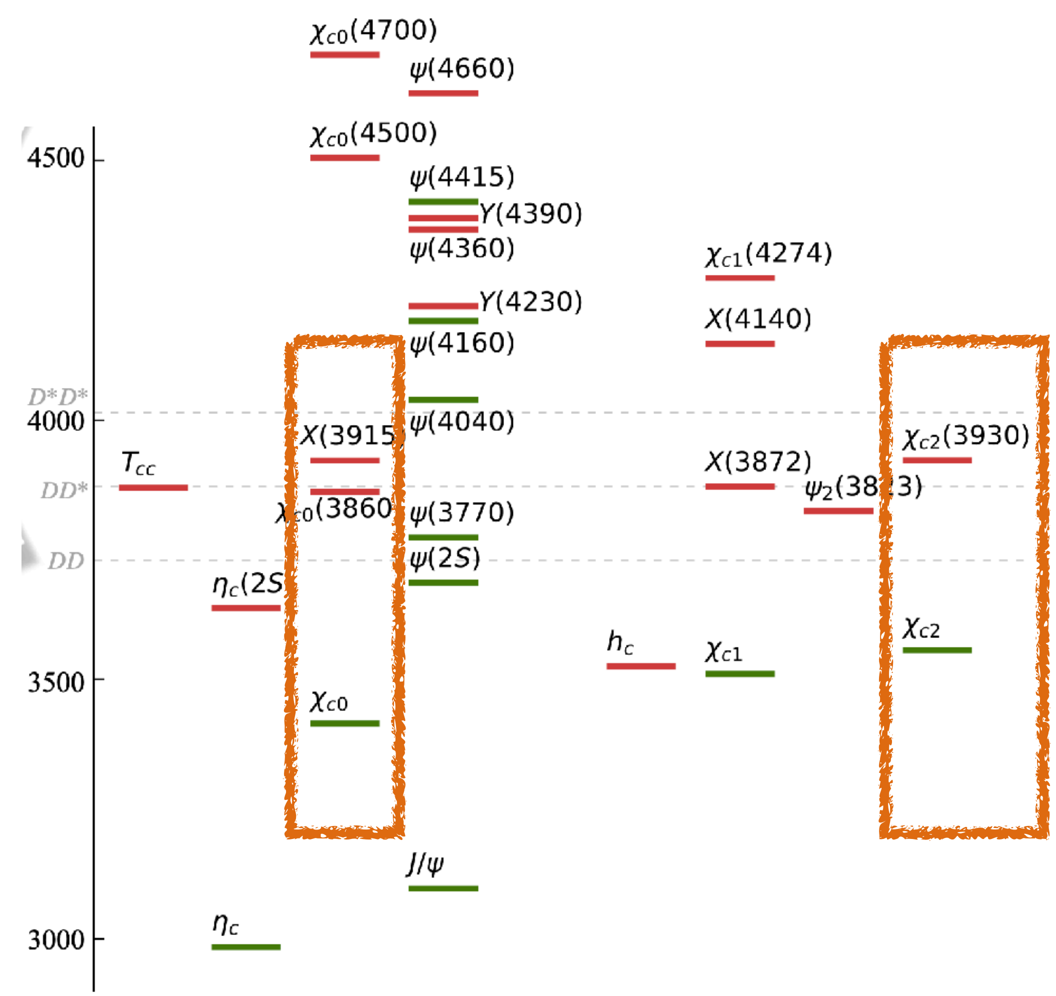
State counting consistent with simple $\bar{c}c$ pictures

No observed "extra" resonances - contrasted theory/ expt

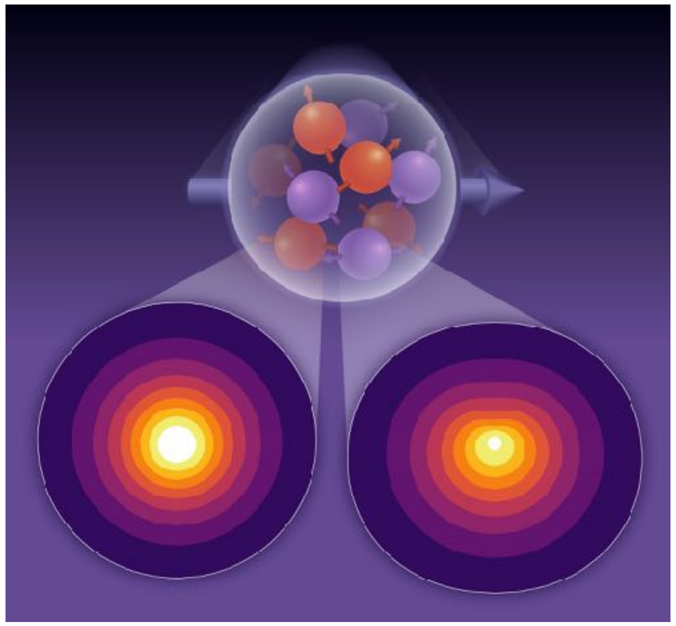
Methods: Graph evaluation techniques developed in partnership with SciDAC RAPIDS

Impact: Mapping charmonium spectrum intense focus in expts. in US, Japan, China, CERN.

Results suggests other particle production methods essential to resolve expt. picture



A Room with a View (of the proton)



u-quark
spatial dist

d-quark
spatial dist

Calculations reveal high-resolution view of quarks inside protons

Phys.Rev.D 106, 114512 & PHYS.ORG

This graphic illustrates a proton moving at nearly the speed of light toward the viewer with its spin aligned along the horizontal direction (large arrow). The two views of concentric circles at the bottom show the spatial distributions of the momentum of up quarks (left) and down quarks (right) within this proton (white is high; violet is low).

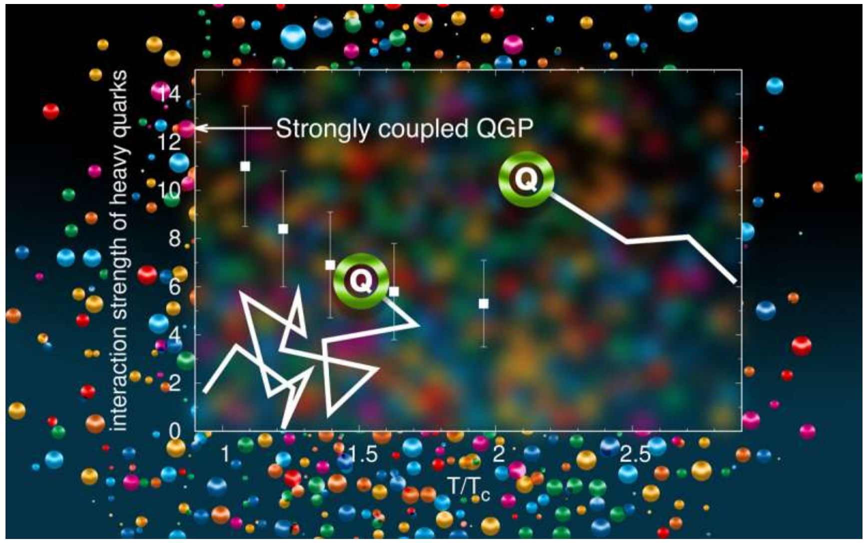
Goal: Map forces from quarks & gluons - origin of mass and spin

Accomplishment: Calculations predict differences of properties of “up” and “down” quarks in proton encoded in Generalized Parton Distribution functions.

Methods: Analysis methods developed under SciDAC.

Impact: Key focus of experiments at JLab12.

Heavy quark diffusion coefficients



Calculation shows why heavy quarks get caught up in the flow

Phys.Rev.Lett. 132 (2024) 5, 051902 & PHYS.ORG

Accomplishment: First calculation of heavy quark diffusion coefficient - describes how quickly a melted soup of quarks & gluons transfer momentum to heavy quarks.

Methods: Analysis methods developed under SciDAC.

Impact: Provides explanation how quark-gluon plasma is a near perfect liquid, first discovered at RHIC (BNL).

SciDAC Goals - Gauge field generation

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

Three pronged research direction with FastMath and RAPIDS:

- Machine-learning for gauge generation
- Hierarchical gauge integration of correlation functions
- Algorithmic improvements in existing stack

SciDAC Goals - Gauge field generation with ML

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

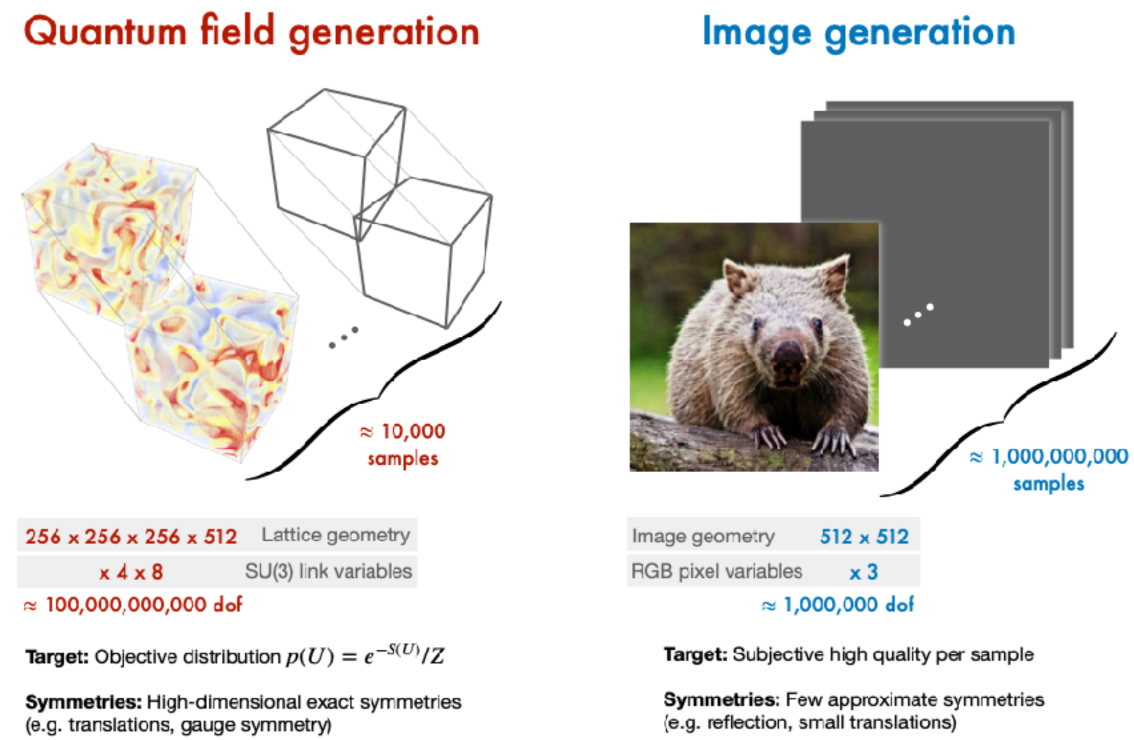
Importance: Future spectroscopy and structure projects need increased fidelity – smaller lattice spacings and much larger statistics

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

Three pronged research direction with FastMath and RAPIDS:

- Machine-learning for gauge generation
- Hierarchical gauge integration of correlation functions
- Improved analysis methods

Incorporate ML techniques into gauge generation, including ML preconditioners (RAPIDS)



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

See talk by Prasanna Balaprakash & posters

SciDAC Goals - Hierarchical gauge generation & integration

Combine gauge generation and measurements

Divide lattice into subdomains & integrate each independently

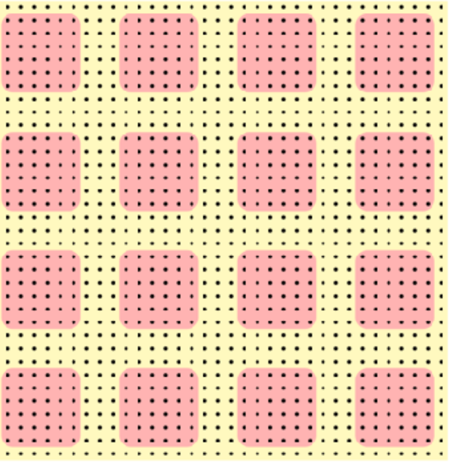
Can lead to 100x to 1000x statistics improvements

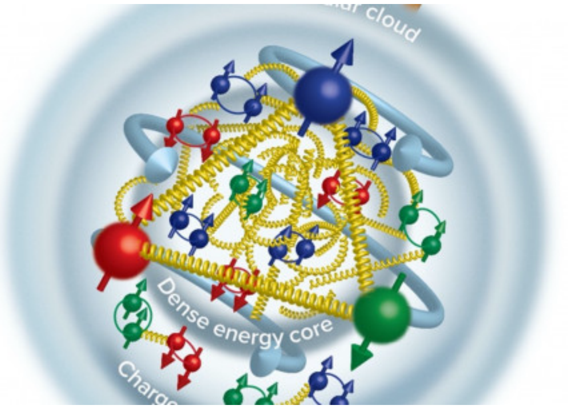
Complications: requires careful attention to quark fermion determinant

Partnership with FastMath includes improved Solvers

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

Disconnected subdomains (red) - buffers (yellow)





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

See talk by Sherry Li & poster

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

SciDAC
Scientific Discovery through Advanced Computing

The details…

Progress during SciDAC-4 - two channel systems

Lattice calculations in finite-volume

Scattering formalism relates finite-volume energies to scattering amplitudes

Multi-channel scattering matrix

solutions, E_n, of

$$\det\left[\mathbf{1} + i\boldsymbol{\rho}\cdot\mathbf{t}\cdot(\mathbf{1} + i\boldsymbol{\mathcal{M}})\right] = 0$$

$\boldsymbol{\rho}(E)$ phase-space

$\mathbf{t}(E)$ scattering matrix

$\boldsymbol{\mathcal{M}}(E,L)$ finite-volume function

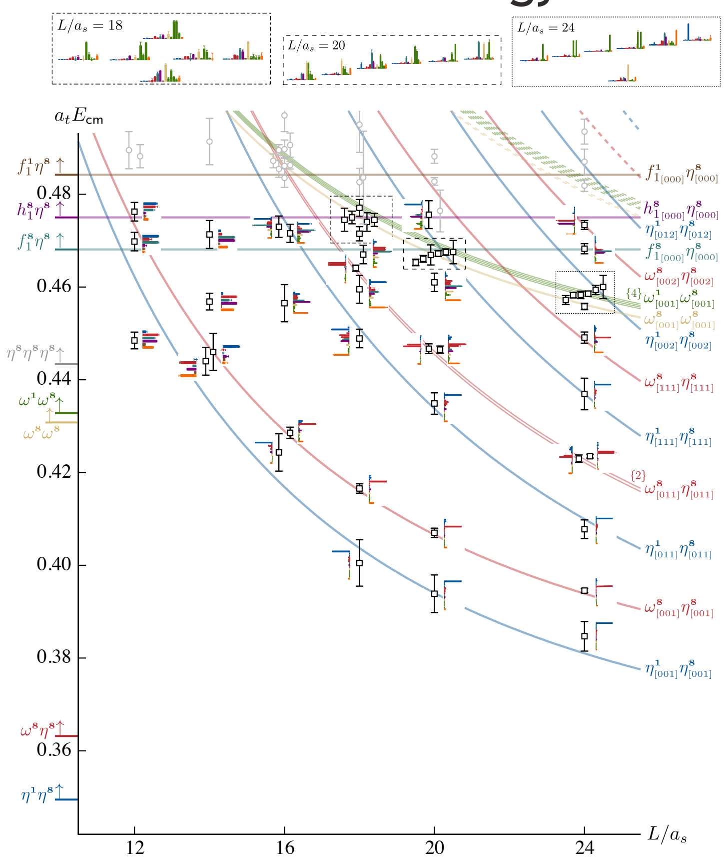
Rigorous for two-body decays

Tackle a real problem in a version of QCD

Compute decay couplings

First prediction for exotic π_1 full width from LQCD

Finite-volume energy levels



Scattering formalism relates finite-volume energies to scattering amplitudes

8 channel scattering matrix

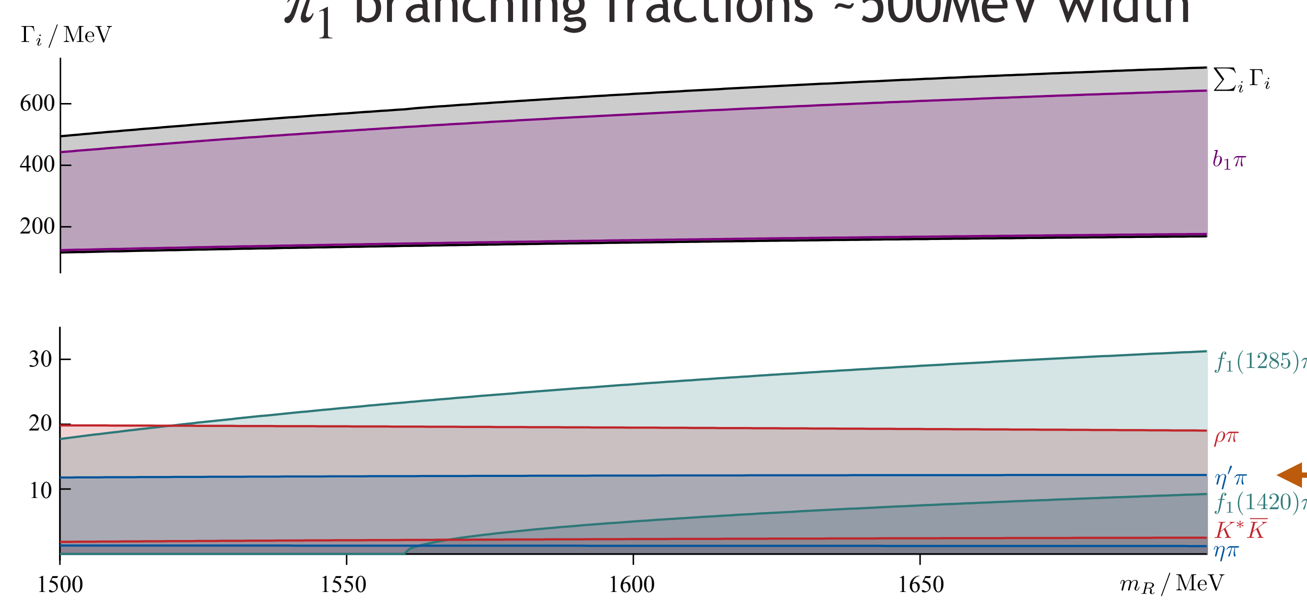
solutions, E_n, of

$$\det\left[\mathbf{1} + i\boldsymbol{\rho}\cdot\mathbf{t}\cdot(\mathbf{1}+i\boldsymbol{\mathcal{M}})\right] = 0$$

$\boldsymbol{\rho}(E)$	phase-space
$\mathbf{t}(E)$	scattering matrix
$\boldsymbol{\mathcal{M}}(E,L)$	finite-volume function

$\pi_1 \to b_1\pi$
$\to \rho\pi$
$\to \eta'\pi$
$\to f_1(1420)\pi$
$\to K^*K$
$\to \eta\pi$

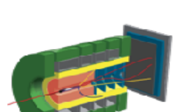
π_1 branching fractions ~500MeV width



$b_1\pi$ much larger than models suggest

GlueX searching here

First determination of full branching fractions for an exotic



GlueX

Jefferson Lab

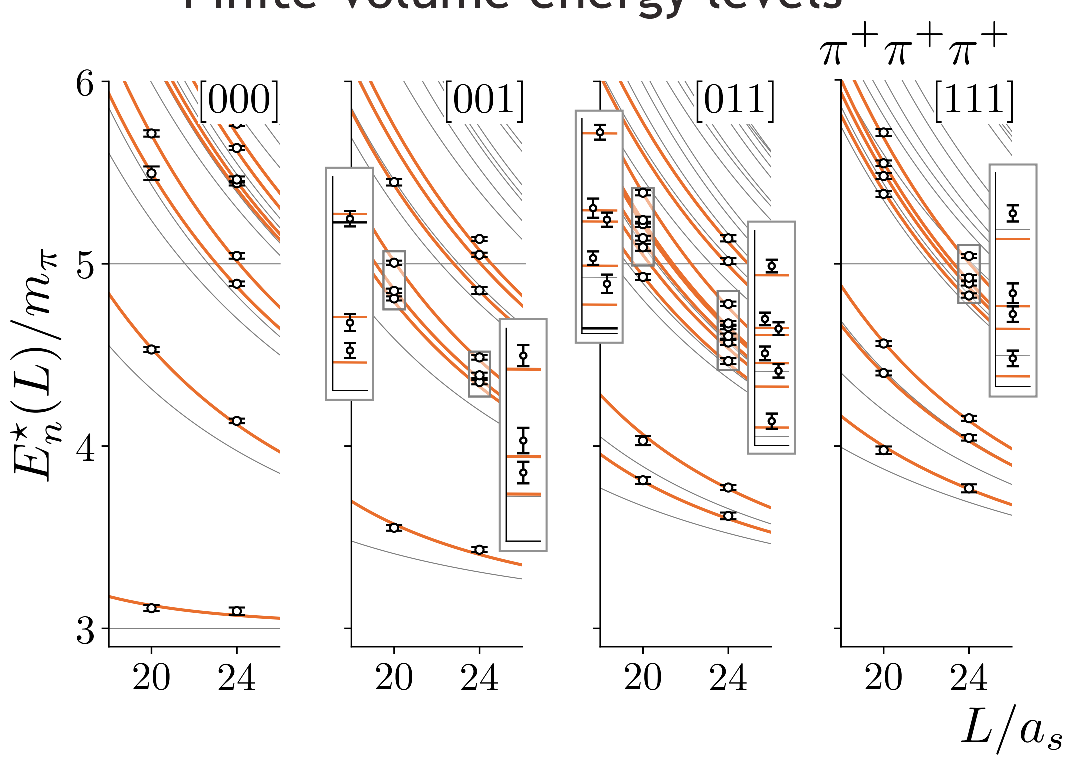
HADRON SPECTRUM: PRD 103

First full 3-body scattering amplitudes QCD

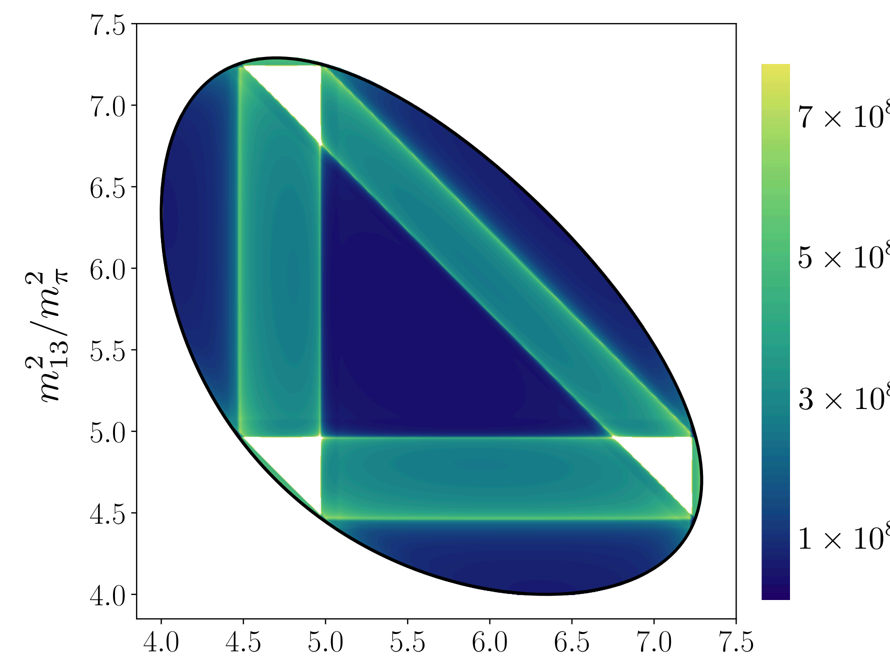
Higher energy states - multi-body decays

More complicated systems, including XYZ-s, are now tractable

Finite-volume energy levels



3-body amplitudes (Dalitz plot)



Hadron Spectrum: PRL 123
Editor's suggestion