Lattice Quantum Chromodynamics Project

SciDAC-4

Robert Edwards
Jefferson Lab

Publicity and useful repositories

GitHub: https://github.com/LQCDSciDAC4 Website: https://lqcdscidac4.github.io

SciDAC
Scientific Discovery through Advanced Computing

LQCD SciDAC-4 Project

Home About Highlights People Publications

LQCD SciDAC-4 Project

The Lattice Quantum Chromo-Dynamics (LQCD) SciDAC-4 Project is supported by the U.S. Dept. of Energy Office of Nuclear Physics and the Office of Advanced Scientific Computing Research. The project is supporting the development of the software infrastructure to carry out scientific calculations to address fundamental questions in nuclear science. It is a collaboration of domain scientists, and computer scientists which aims to understand the structure of nuclear matter under extreme conditions, and how quarks and gluons are confined to build the matter that is observed in nature.

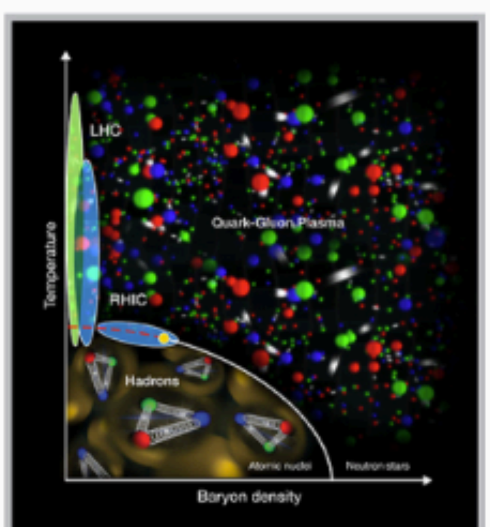
News

SciDAC
Scientific Discovery through Advanced Computing

Exploring the Exotic World of Quarks and Gluons at the Dawn of the Exascale

Jefferson Lab Highlights, 2017-10-11

Jefferson Lab leads development of next-generation software to benefit nuclear physics computation. An award was recently announced by DOE's Office of Nuclear Physics and the Office of Advanced Scientific Computing Research in the Office of Science. It will provide $8.25 million for the "Computing the Properties of Matter with Leadership Computing Resources" research project.



Using Supercomputers to Delve Ever Deeper into the Building Blocks of Matter

Brookhaven National Lab Features, 2017-10-18

Scientists to develop next-generation computational tools for studying interactions of quarks and gluons in hot, dense nuclear matter

LQCD ASCR/NP SciDAC-4

Computing the Properties of Matter with Leadership Computing Resources

PI: Robert Edwards (JLab)

Co-PIs: William Detmold (MIT), Balint Joo (JLab), Swagato Mukherjee (BNL)

Senior Investigators:

Andrei Alexandru (GWU)
Saman Amarasinghe (MIT)
Alexei Bazavov (MSU)
Kate Clark (NVIDIA)
Rob Fowler (UNC)
Dhiraj Kalamkar (Intel)
Xu Liu (W&M Computer Sci)
Kostas Orginos (W&M Phys)
Sergey Panitkin (BNL)
Andrew Pochinsky (MIT)
Kenneth Roche (PNNL)
Martin Savage (UW)
Frank Winter (JLab)
Boram Yoon (LANL)

https://lqcdscidac4.github.io

Team members

Long term collaborations with ASCR supported community and Industry

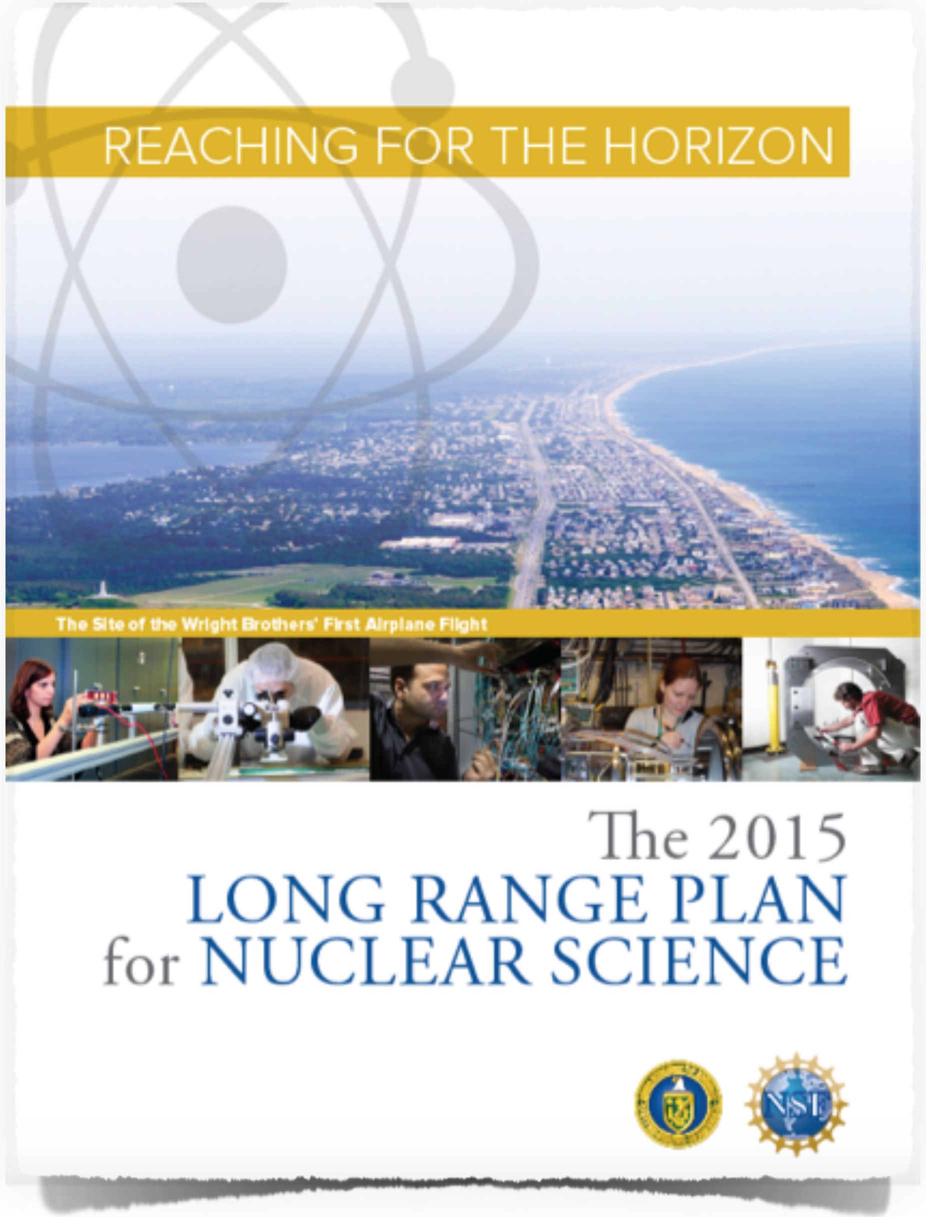
- Gauge generation (co-PI: Balint Joo)
  - Balint Joo/Eloy Romero - Sparse linear system solvers on emerging LCF-s
  - Frank Winter - Chroma & QDP/JIT
  - Boram Yoon - Sympletic PDE Integrators
  - Kate Clark (NVIDIA) - comms reduced solvers, integrators
  - Robert Fowler - QUARC/DSL interface to Clang/LLVM - automatic code generation

- Correlation functions/contractions (co-PI: Will Detmold)
  - Saman Amarasinghe - (TACO) code generation, auto-tuning for contractions (& gauge gen)
  - Andrew Pochinsky - Halide for QCD
  - Eloy Romero - contractions
  - Xu Liu - memory optimizations for contractions (on GPUs)
  - Kostas Orginos - matrix elements
  - Kenneth Roche - workflow, data reductions/sparsification/SVD approximations for contractions
  - Andrei Alexandrou - overlap analysis campaigns for KNL-s

- Thermodynamics and Workflow (co-PI: Swagato Mukherjee)
  - Sergey Panitkin: PanDA/ATLAS workflow for LCF systems, multi-site campaigns, scheduling, file transfers & data integrity
  - Alexei Bazavov - transport coefficients

Science Drivers

Science areas recognized in the 2015 NSAC Long Range Plan

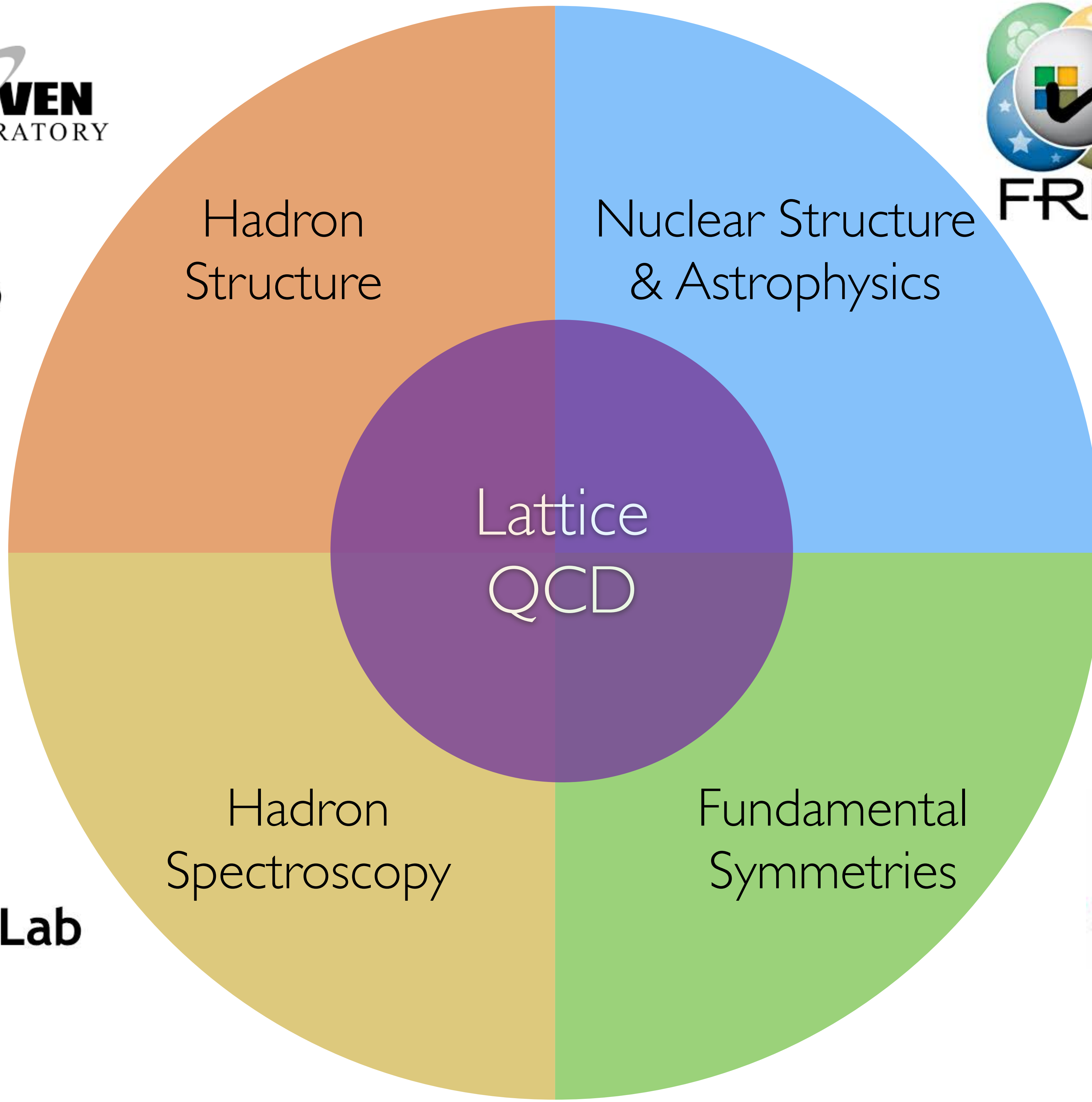


- Extreme matter at high temperatures and/or densities
  - BNL and a future EIC
  - DOE Topical collab. (Mukherjee)
- Hadron spectroscopy
  - CLAS12 & GlueX @ JLab
- Hadron structure
  - JLab, RHIC-Spin @ BNL, future EIC
  - DOE Topical collab. (J.W. Qiu & W. Detmold)
- Nuclear structure and interactions
  - FRIB, components of SM tests at JLab
- Tests of fundamental symmetries
  - Violations of SM, parity violating expts, proposed new low-energy facilities

Hadrons and Nuclei

BROOKHAVEN NATIONAL LABORATORY

Jefferson Lab



FRIB

DUNE

Argonne NATIONAL LABORATORY

Los Alamos NATIONAL LABORATORY

SNS SPALLATION NEUTRON SOURCE

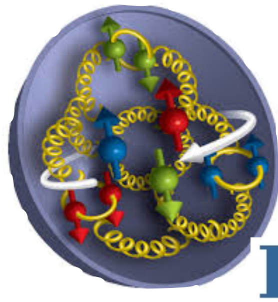
Jefferson Lab

Jefferson Lab

LQCD/NP Science & connection to Expt.

PHENIX

STAR



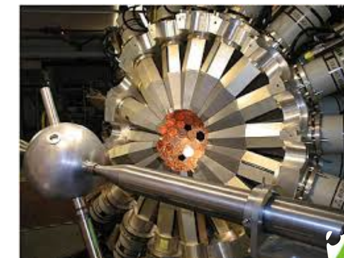
RHIC

Jefferson Lab

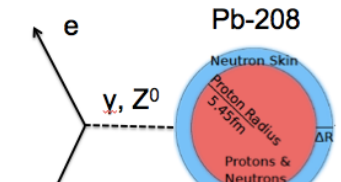
SeaQuest E906

DUNE

FAIR
Facility for Antiproton and Ion Research in Europe GmbH

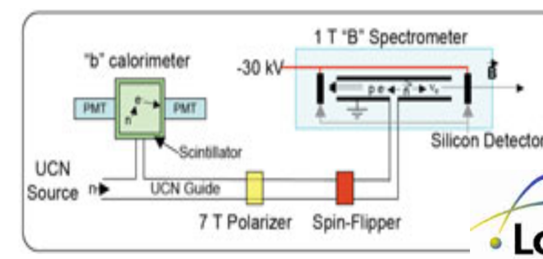


Argonne NATIONAL LABORATORY



PREX II

FRIB



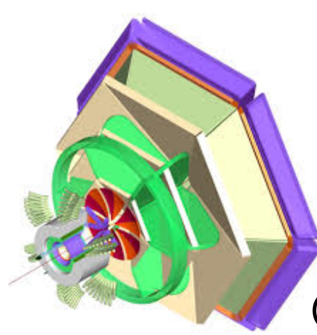
Los Alamos NATIONAL LABORATORY

BESIII

LHCb

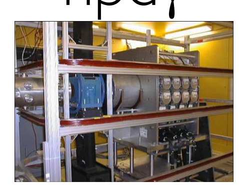
Belle II

GlueX



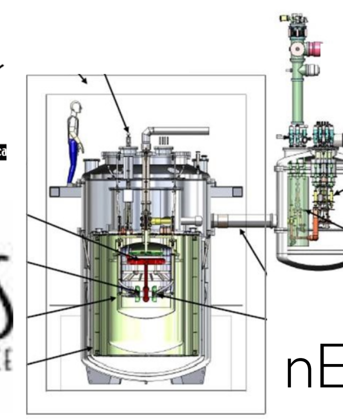
CLAS12

npdγ



Enriched Xenon Observatory for double beta decay

SNS SPALLATION NEUTRON SOURCE



nEDM

PAUL SCHERRER INSTITUT PSI

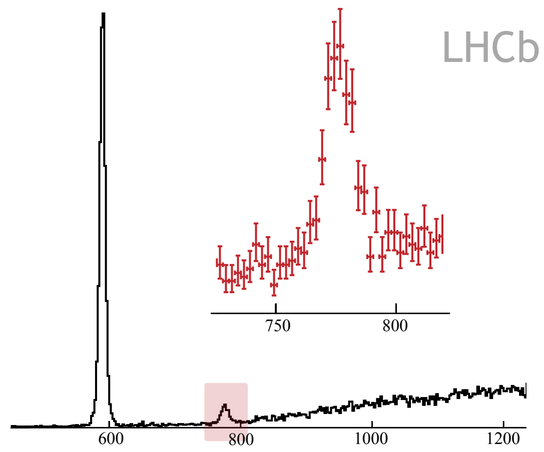
MuSUN

QCD, hadrons and the standard model

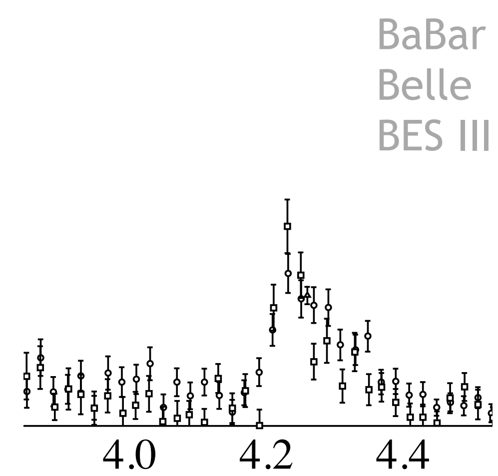
While **QCD** may be a solid part of the **standard model**, and **hadrons** are ubiquitous in HEP experiments, there remain significant mysteries in how **hadrons** are built from **quarks** and **gluons**

unexpected ?

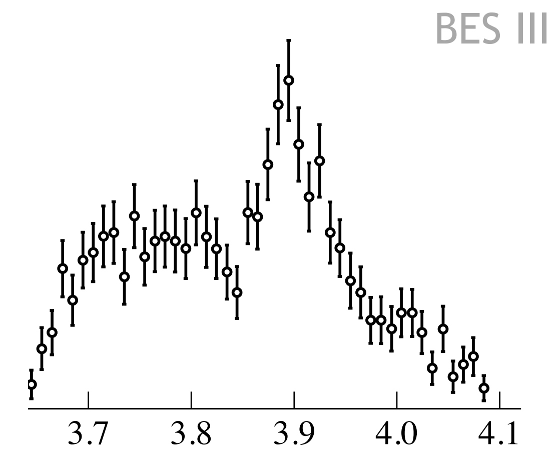
$X(3872) \to \pi\pi J/\psi$



$Y(4260) \to \pi\pi J/\psi$



$Z_c(3900) \to \pi^+ J/\psi$



QCD, hadrons and the standard model

While **QCD** may be a solid part of the **standard model**, and **hadrons** are ubiquitous in HEP experiments, there remain significant mysteries in how **hadrons** are built from **quarks** and **gluons**

unexplained ?

light scalar meson resonances

$\boxed{f_0(500) \text{ or } \sigma}$ [g] was $f_0(600)$ $\quad I^G(J^{PC}) = 0^+(0^{++})$

Mass $m = (400\text{–}550)$ MeV
Full width $\Gamma = (400\text{–}700)$ MeV

$\boxed{f_0(980)}$ [j] $\quad I^G(J^{PC}) = 0^+(0^{++})$

Mass $m = 990 \pm 20$ MeV
Full width $\Gamma = 10$ to 100 MeV

$\boxed{K_0^*(800)}$ or κ $\quad I(J^P) = \frac{1}{2}(0^+)$

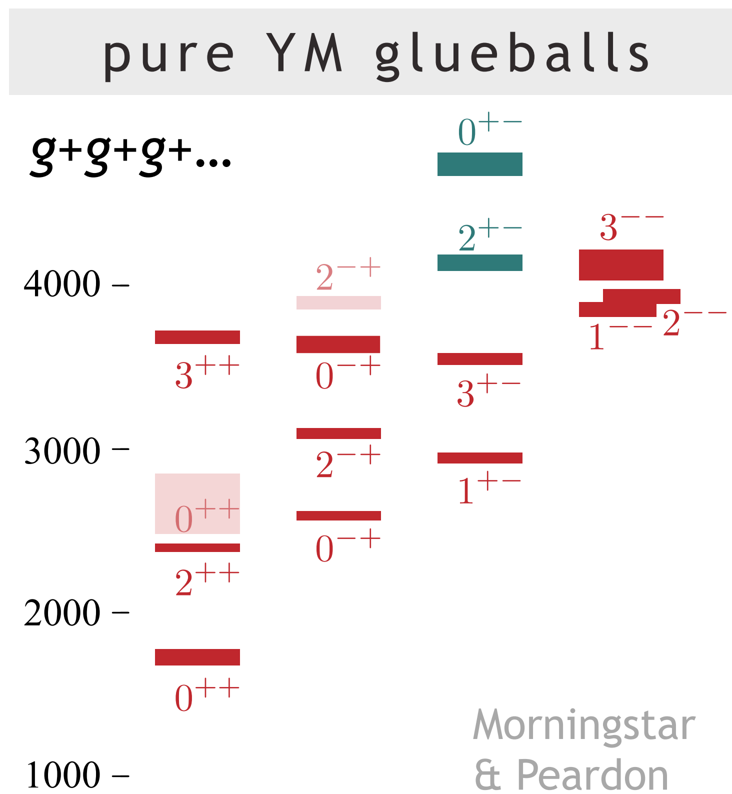
$\boxed{a_0(980)}$ [j] $\quad I^G(J^{PC}) = 1^-(0^{++})$

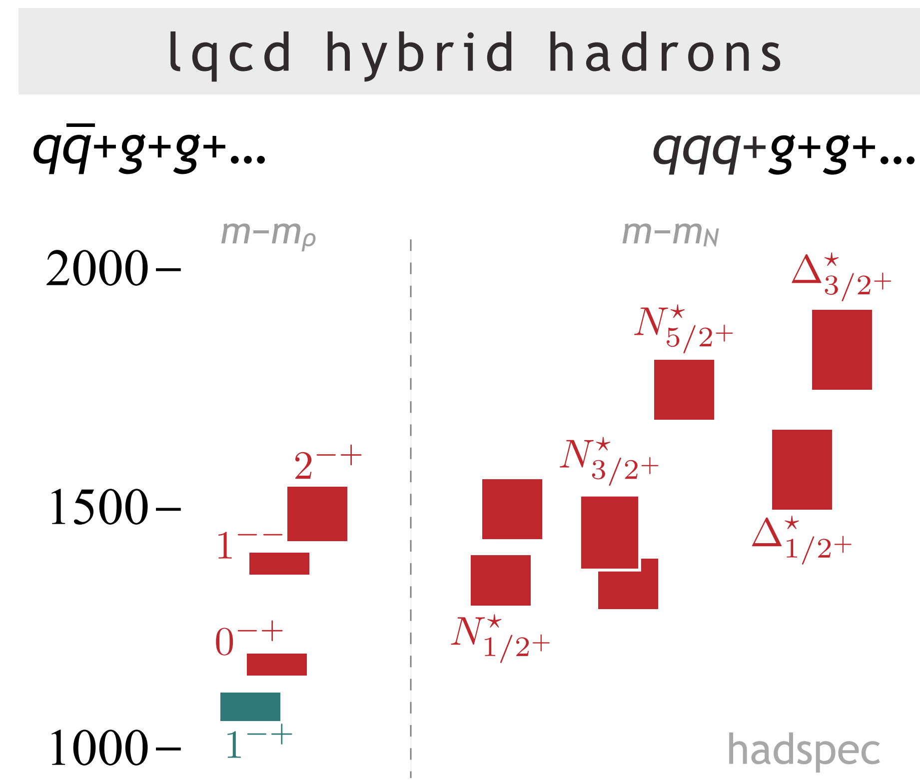
Mass $m = 980 \pm 20$ MeV
Full width $\Gamma = 50$ to 100 MeV

QCD, hadrons and the standard model

While **QCD** may be a solid part of the **standard model**, and **hadrons** are ubiquitous in HEP experiments, there remain significant mysteries in how **hadrons** are built from **quarks** and **gluons**

unobserved ?

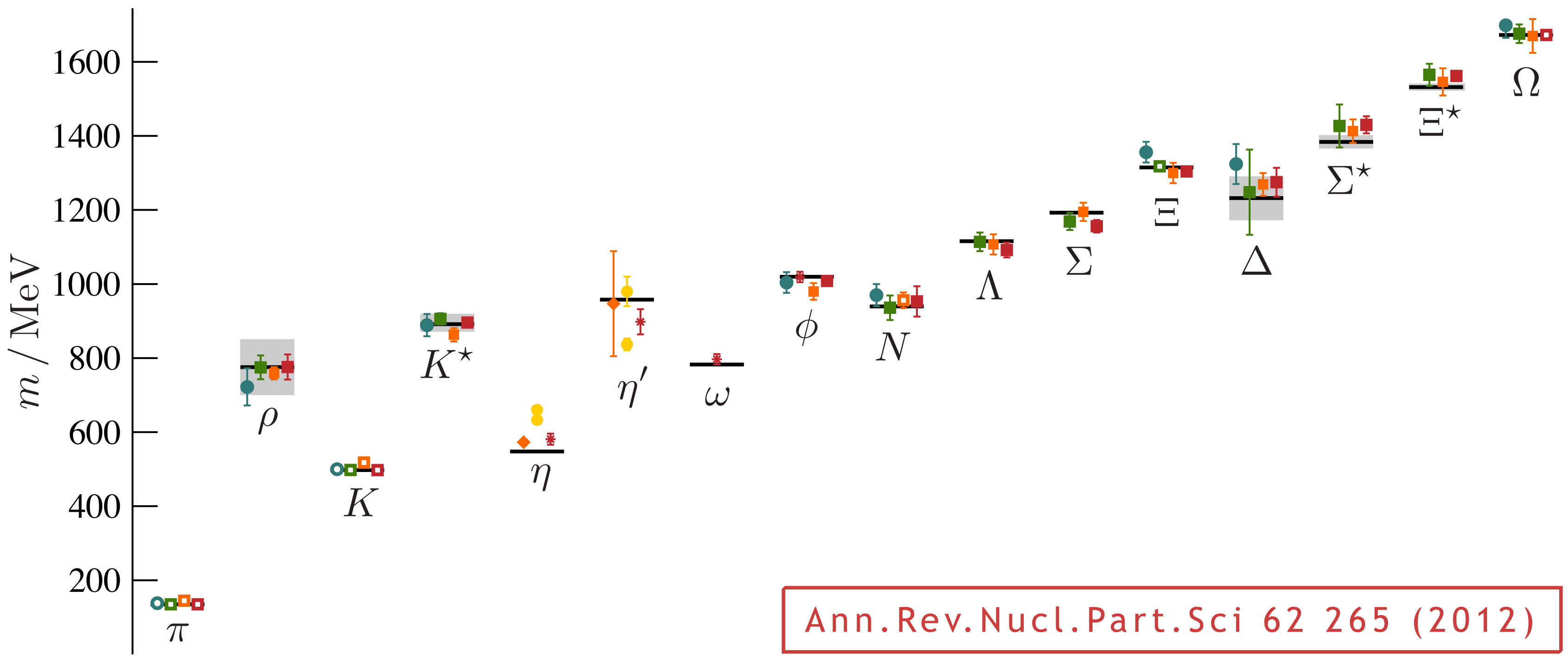




Jefferson Lab

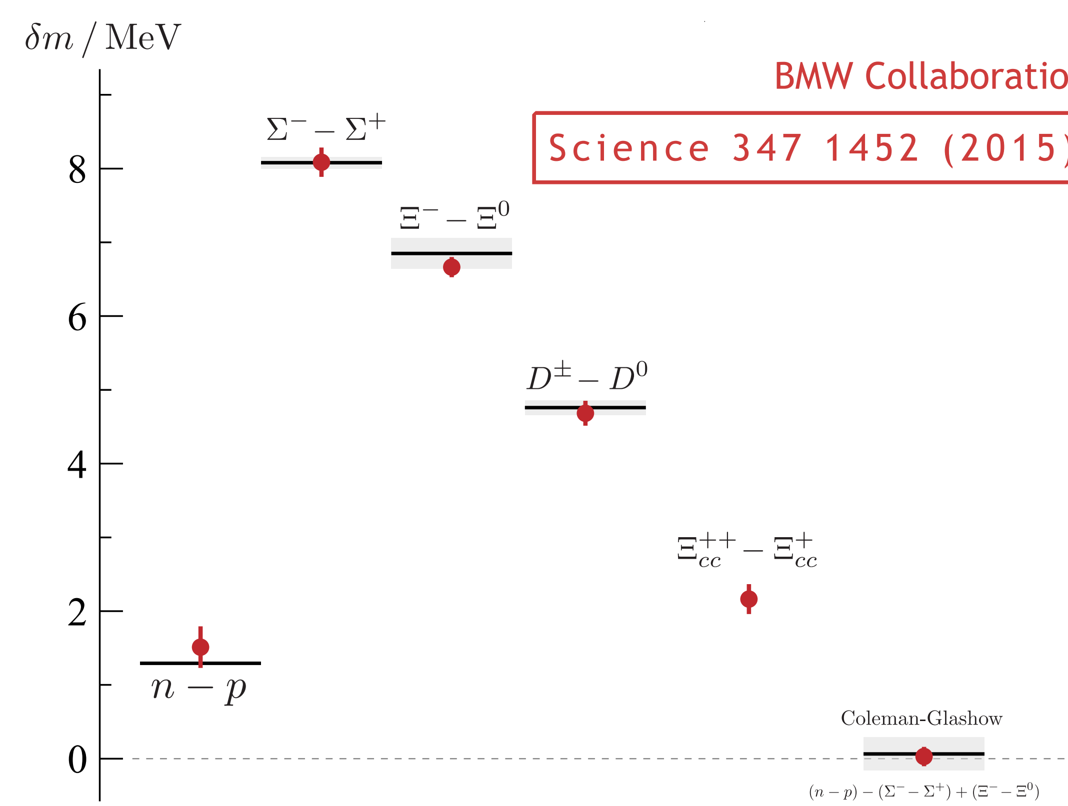
Precise spectroscopy of stable hadrons

lattice qcd light hadron spectrum



Ann.Rev.Nucl.Part.Sci 62 265 (2012)

QCD+QED mass shifts



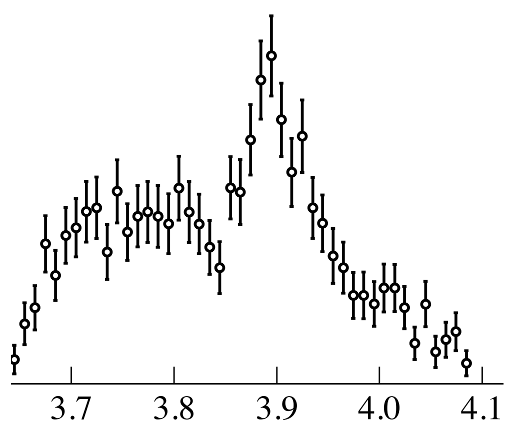
Science 347 1452 (2015)

Excited spectroscopy

but much of the excitement in hadron spectroscopy is in **heavier states**

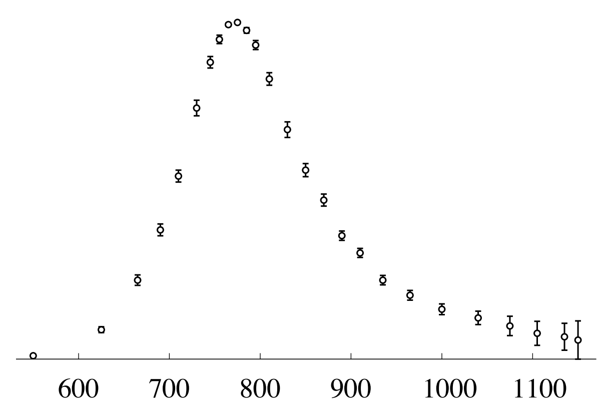
and they are **resonances** observed through their decays

$Z_c(3900) \rightarrow \pi^+ J/\psi$



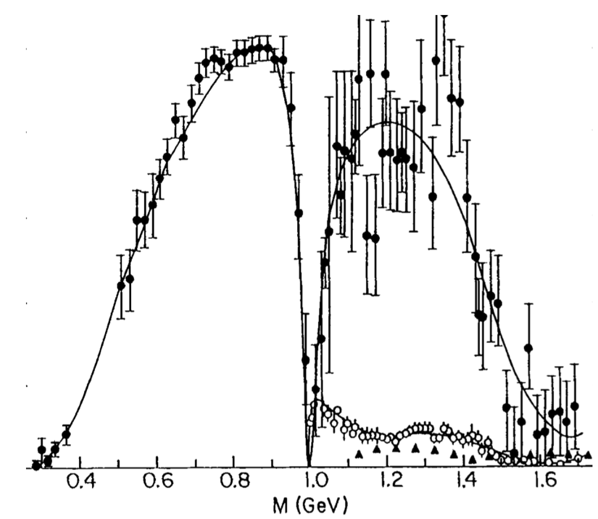
exotic

$\rho \rightarrow \pi\pi$



familiar

$\pi\pi \rightarrow \pi\pi, K\bar{K}, \eta\eta$



non-trivial

same non-perturbative dynamics **binds** and causes the **decay** — can't be separated within QCD …

a faithful QCD calculation should give **all the scattering physics** at once …

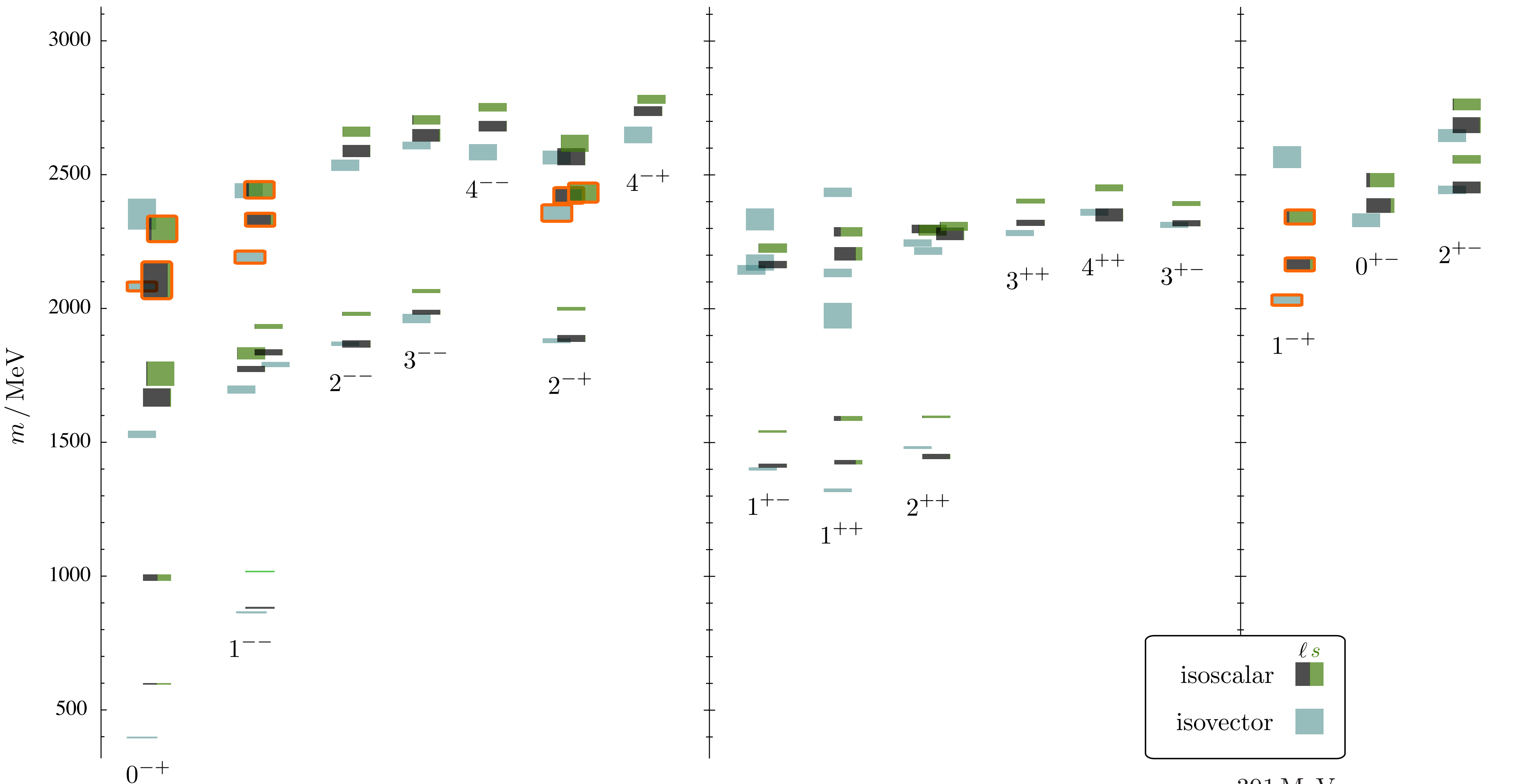
Lattice QCD & the excited meson spectrum

LQCD SciDAC project has pioneered novel techniques in lattice QCD

Featured in Particle Data Group

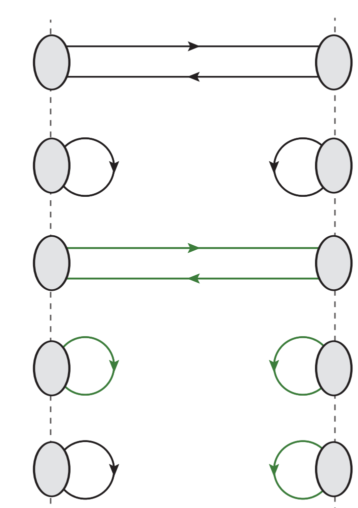
Light quark meson + "exotics" & "hybrids" spectrum

Exotics



$m_\pi \sim 391\,\mathrm{MeV}$

'Toward the excited isoscalar meson spectrum from lattice QCD'
PRD 88 094505 (2013)



high precision calculation of **disconnected diagrams**

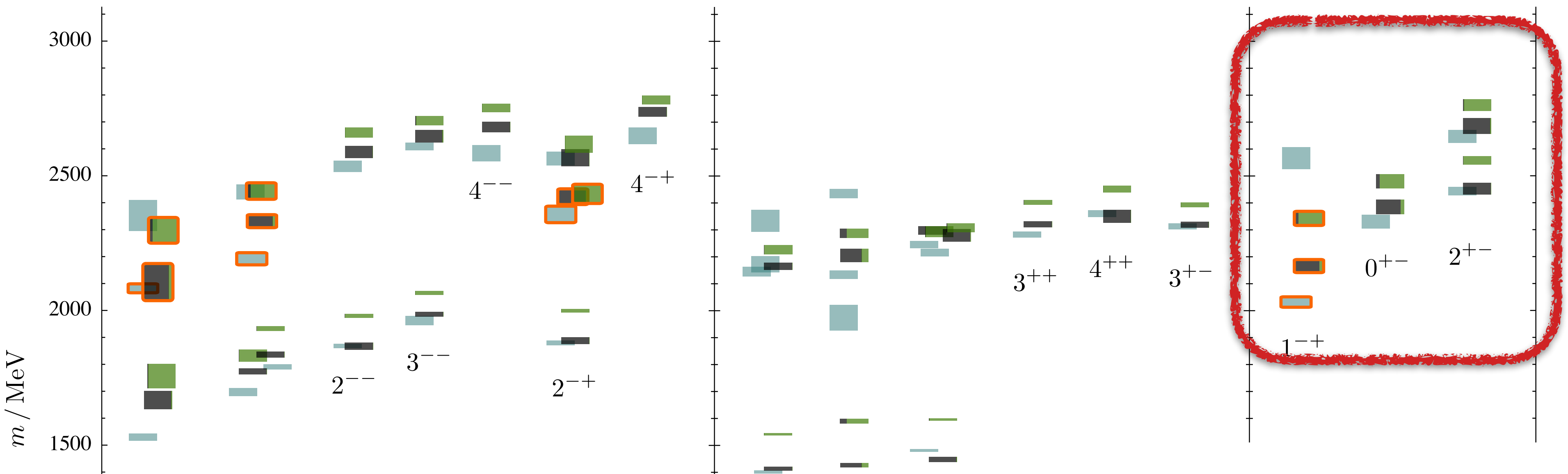
clear indication of a spectrum of **hybrid mesons**

early adopters of GPUs

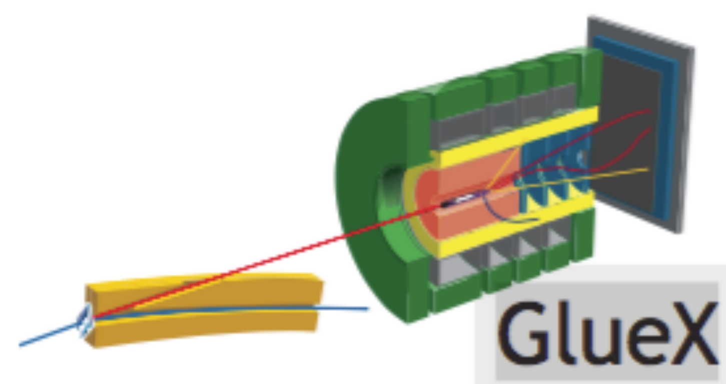
Hadron Spectroscopy - role of the glue

Light quark meson + “exotics” & “hybrids” spectrum

Exotics



Clear indication of exotics



But missing key info

- ➡ Need to know decay modes and rates to compare to expt.
- ➡ Major focus of program

Where are the "Missing" Baryon Resonances?

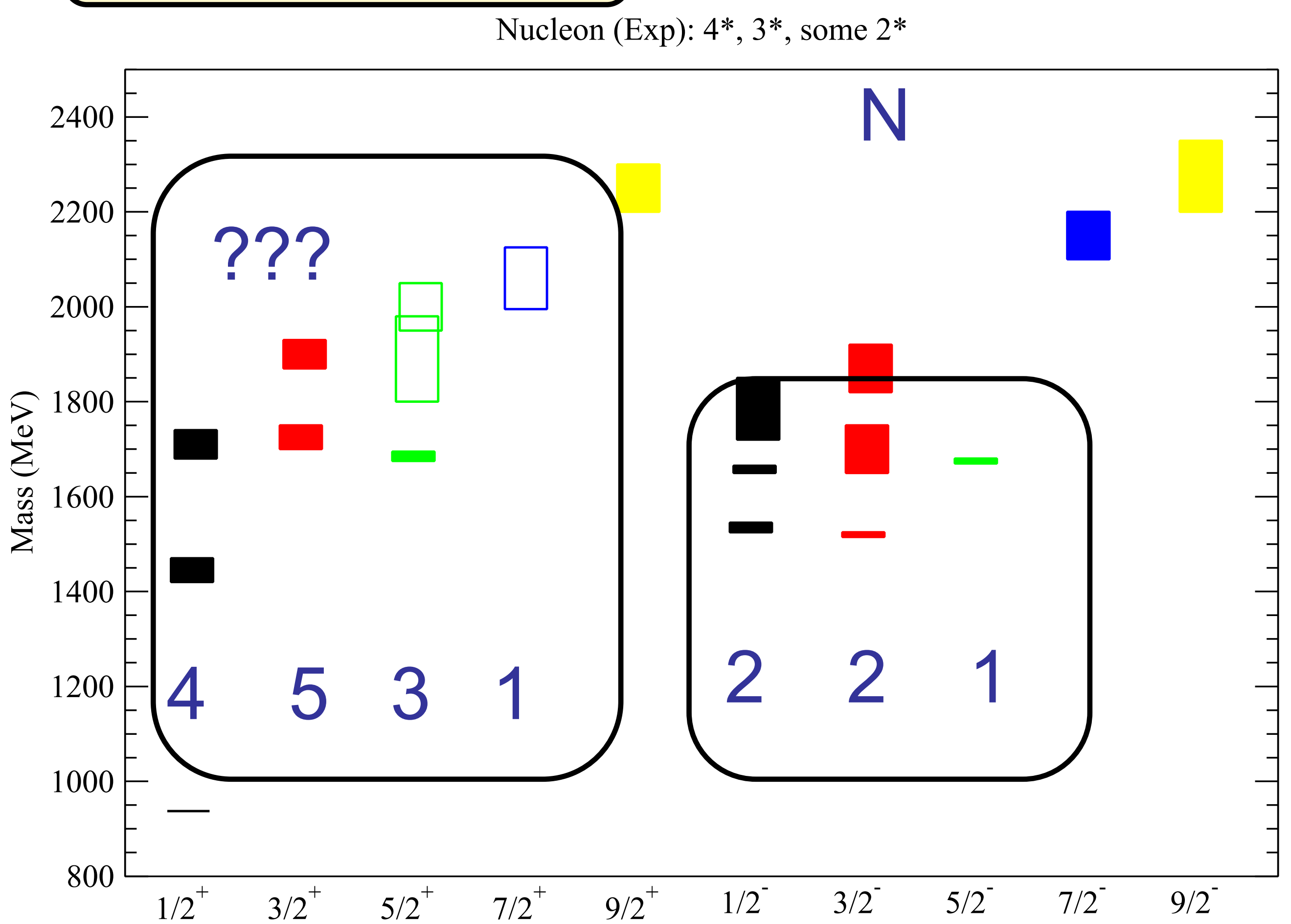
Only few found in expt. - thought that they were missing?

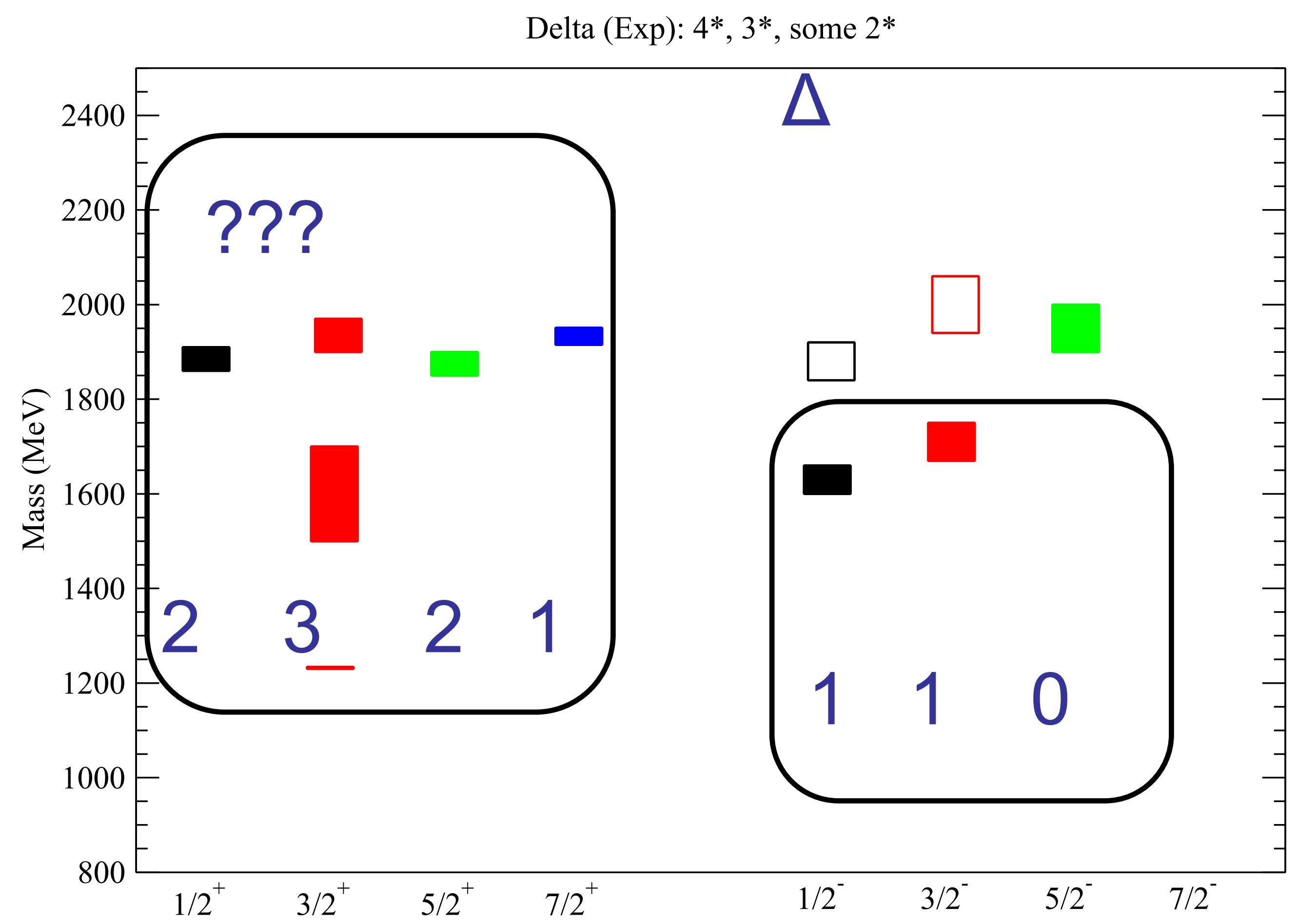
Theory/symmetries wrong?

Nucleon & Delta spectrum

PDG uncertainty on
B-W mass

Expt. vs. predictions



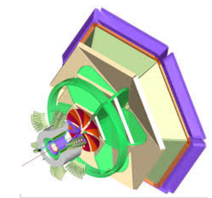


Jefferson Lab

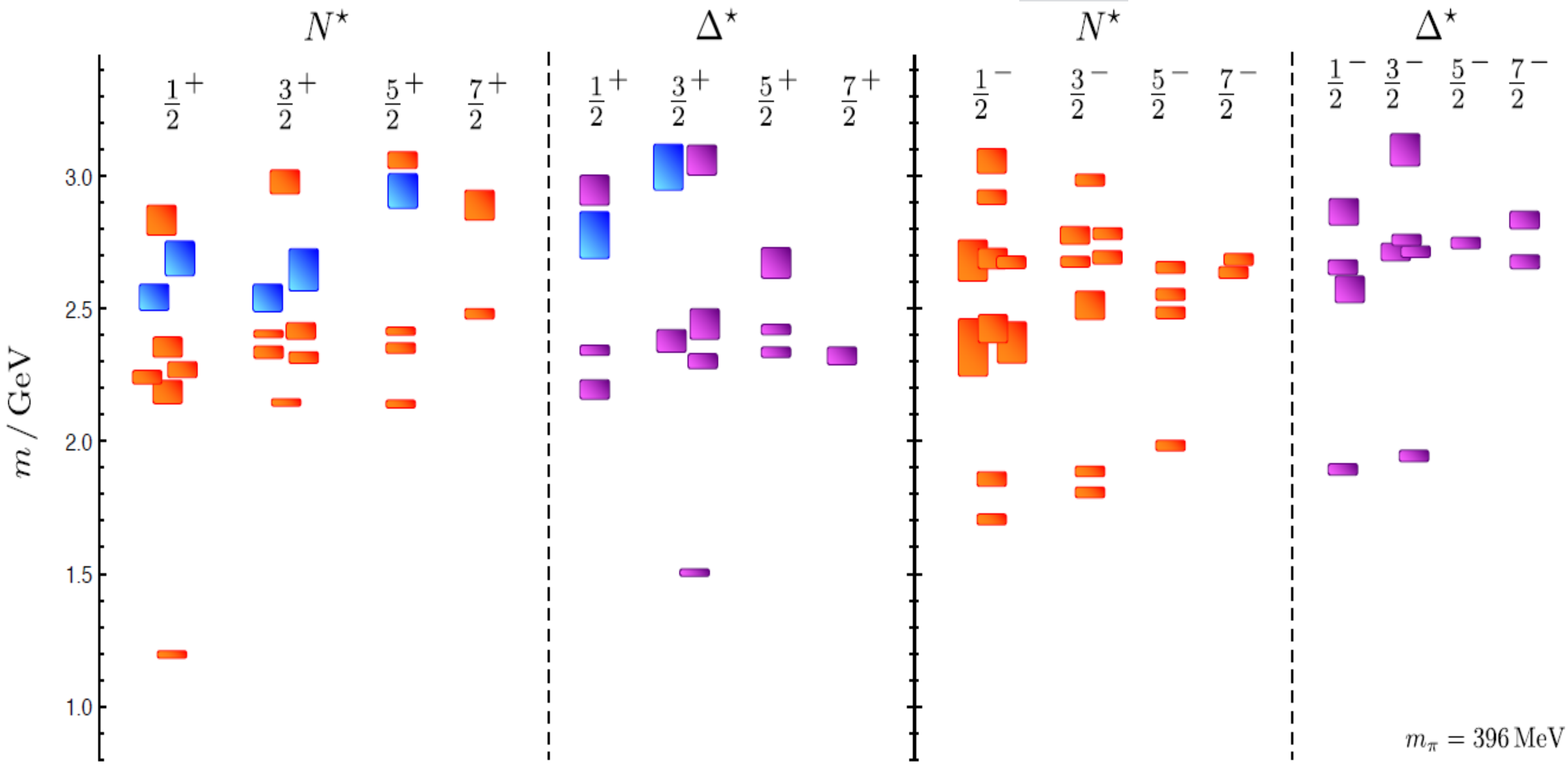
LQCD sees rich spectrum, including hybrids

Featured in Particle Data Group

Focus of CLAS12 @ JLab & Bonn & Mainz & LHCb @ CERN



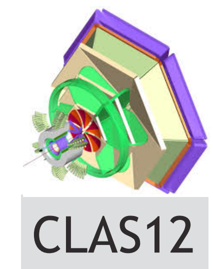
CLAS12



LQCD suggest no “missing" baryon states

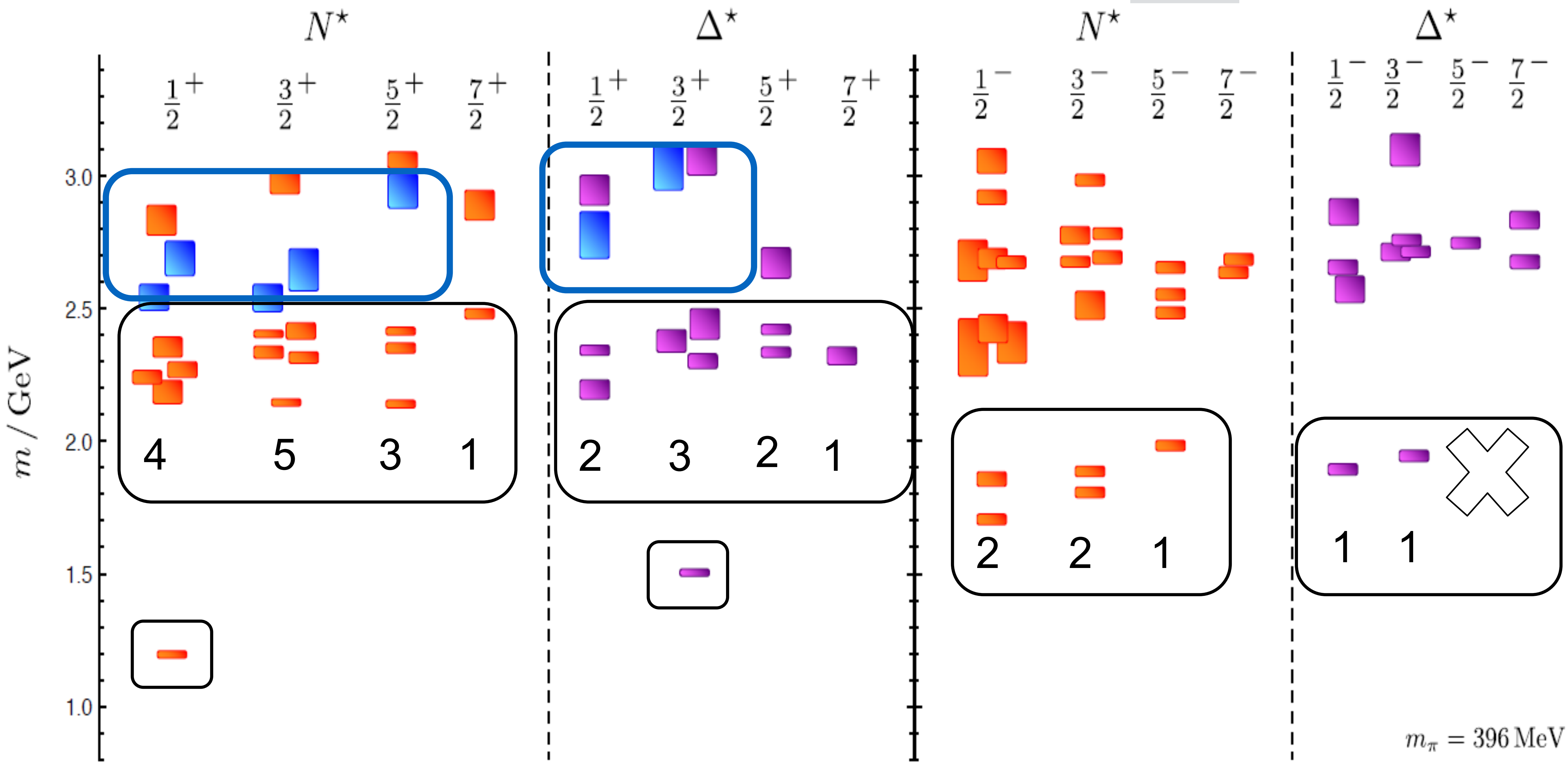
Focus of CLAS12 @ JLab & Bonn & Mainz & LHCb @ CERN

Featured in Particle Data Group



Additional gluonic excitations within baryons

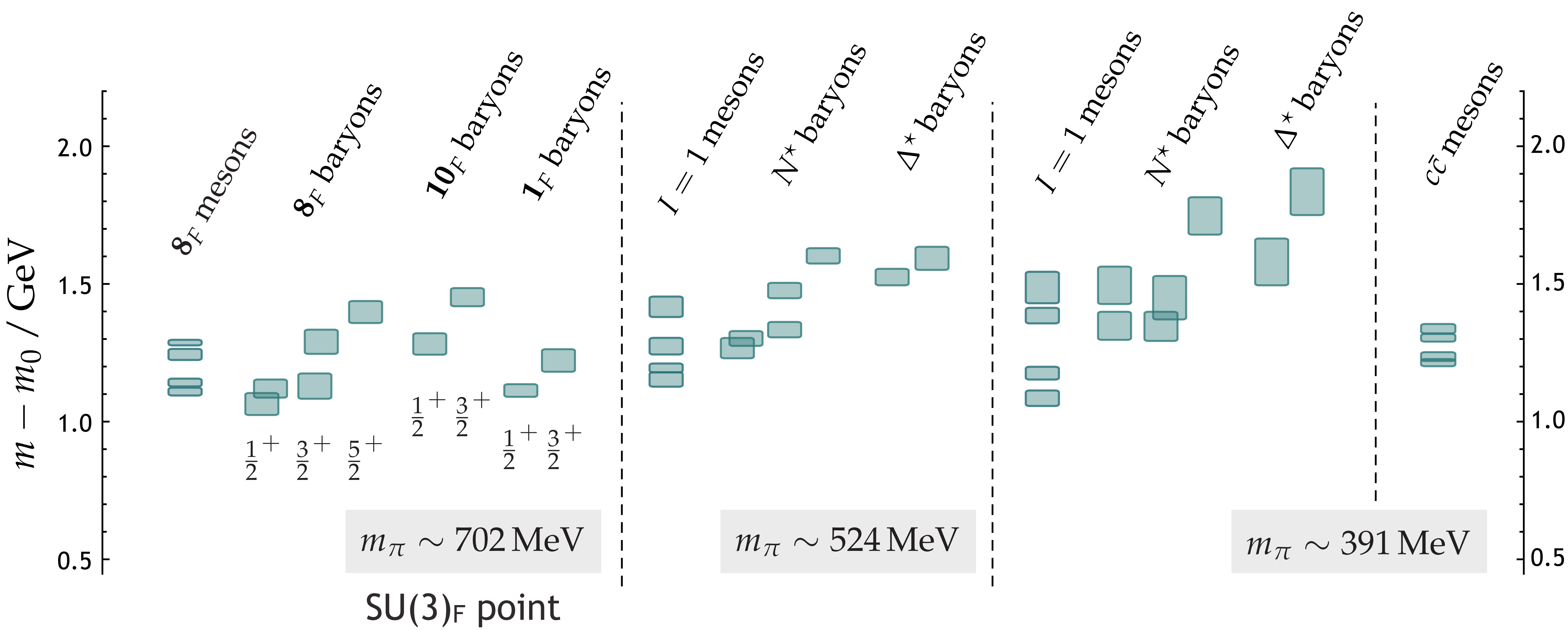
Spurred new expt. search in CLAS12@JLab



➡ Need observations in more decay channels

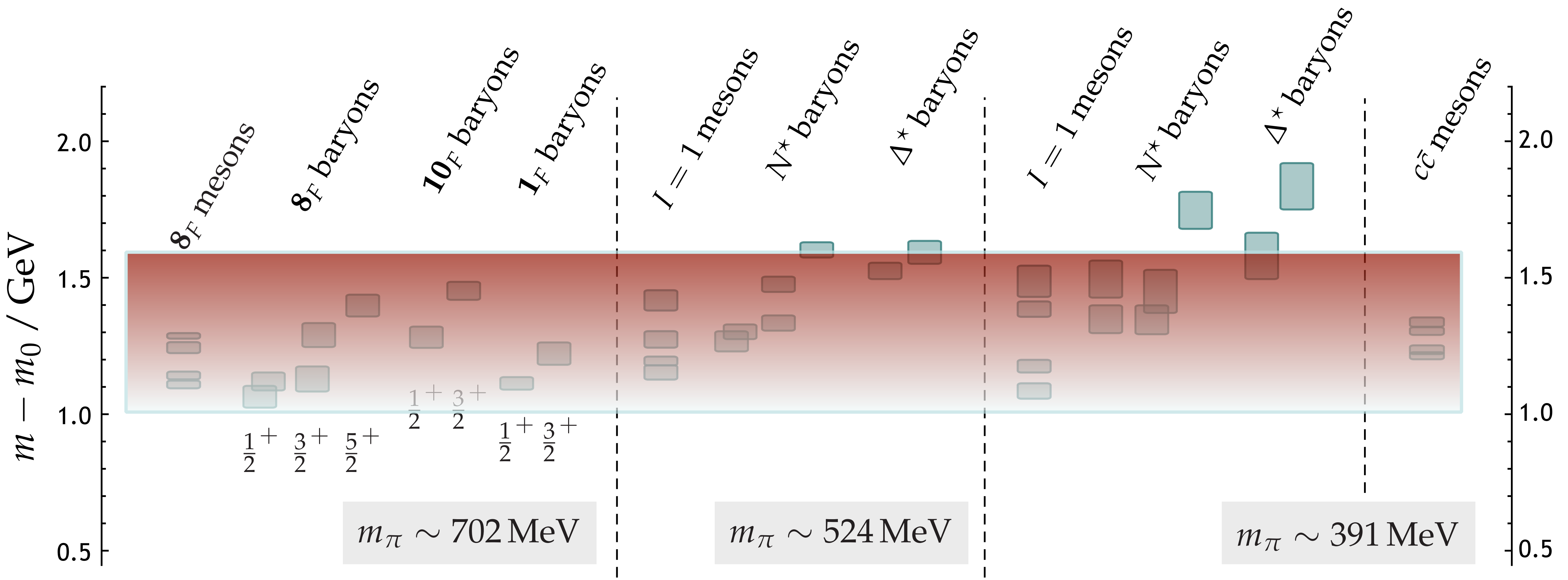
Hadron Spectroscopy - role of the glue

- Subtract the 'quark mass' contribution

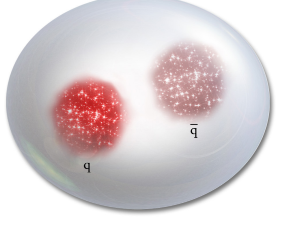


Hadron Spectroscopy - role of the glue

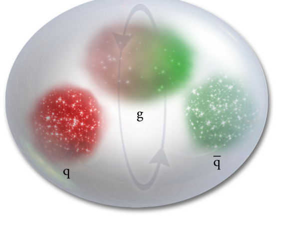
- Subtract the ‘quark mass’ contribution



SU(3)F point



Conventional Meson

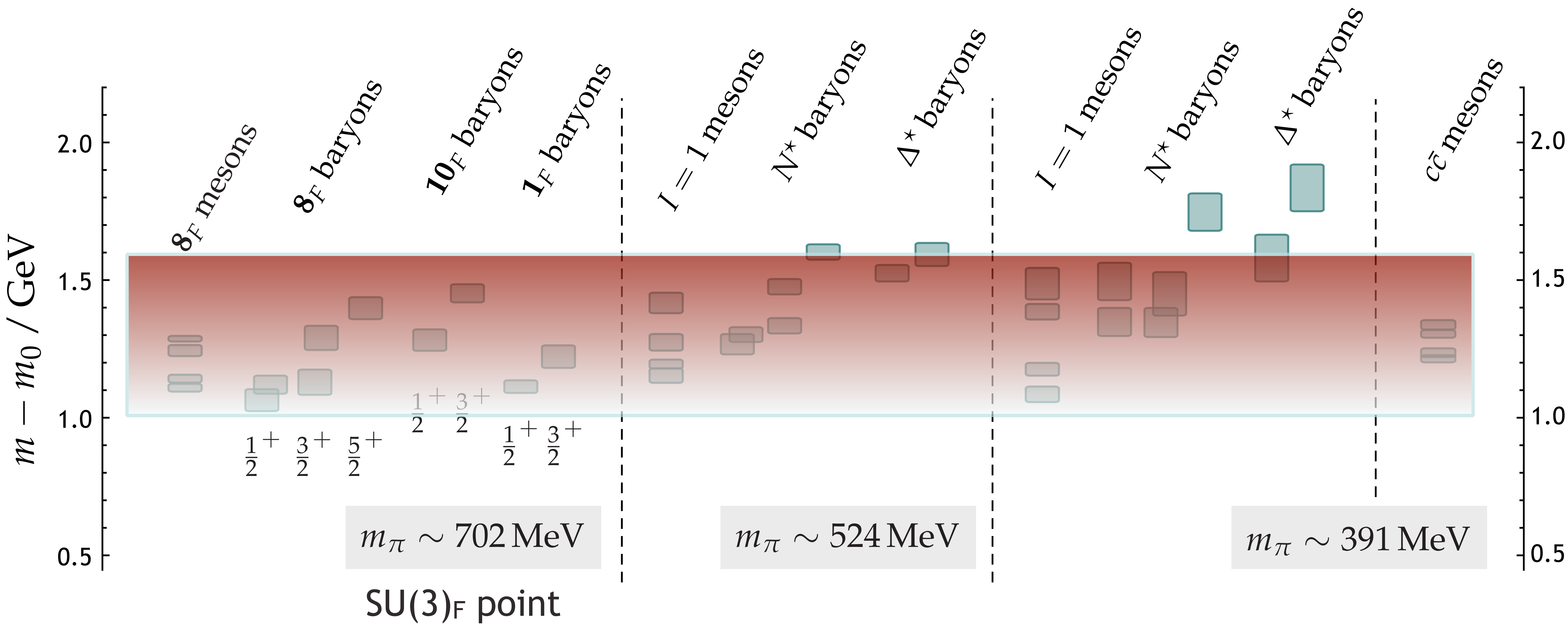


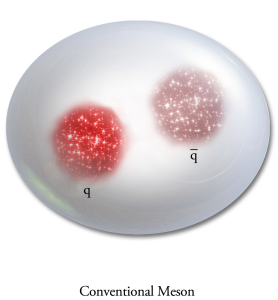
Hybrid Meson

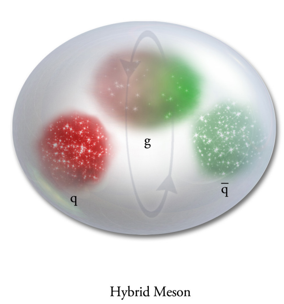
Common energy scale of gluonic excitation ~ 1.3 GeV

Hadron Spectroscopy - role of the glue

- Subtract the ‘quark mass’ contribution







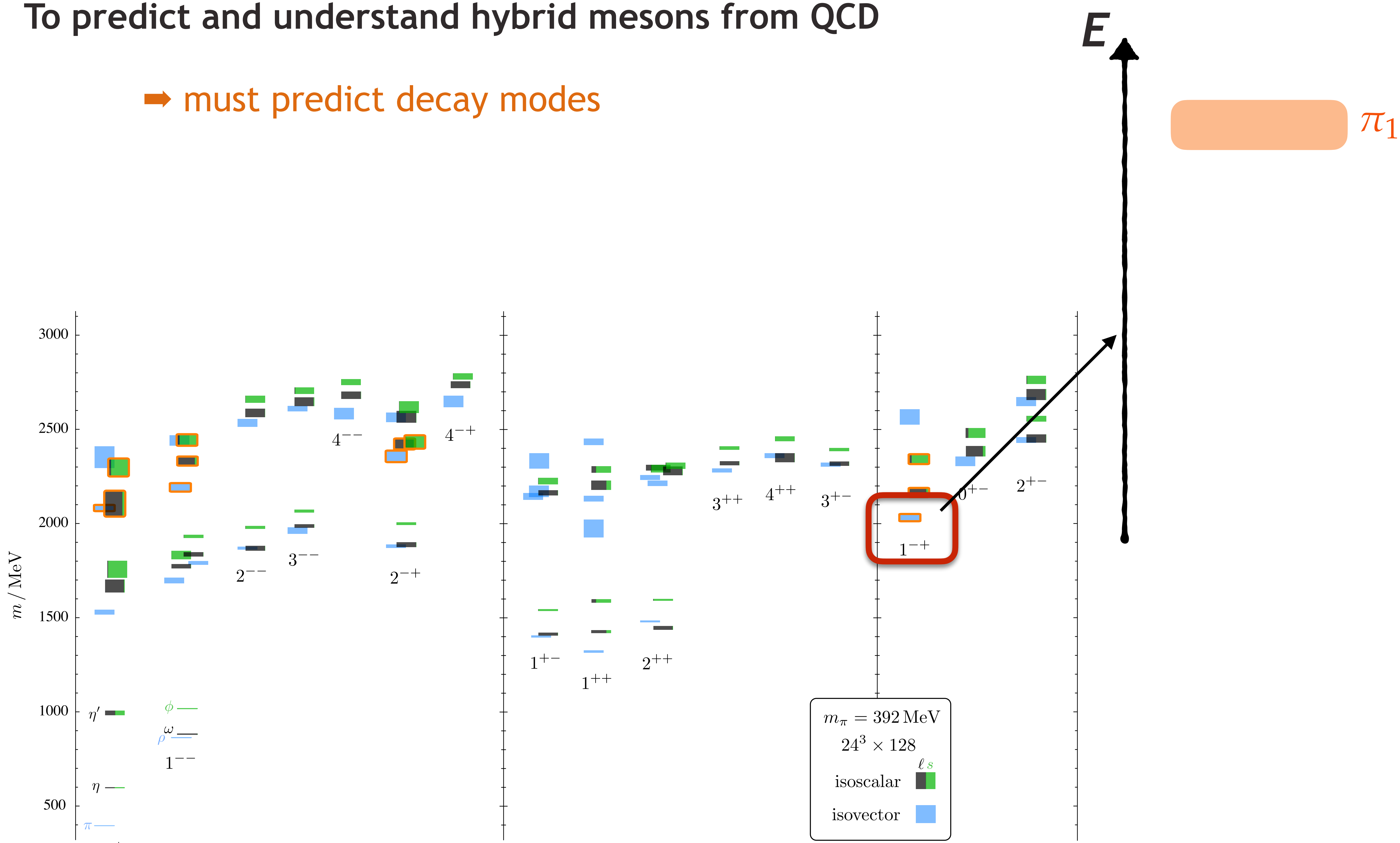
Common energy scale of gluonic excitation ~ 1.3 GeV

Should have measurable effects in hadron structure

Exotic hybrid mesons in QCD?

To predict and understand hybrid mesons from QCD

➡ must predict decay modes



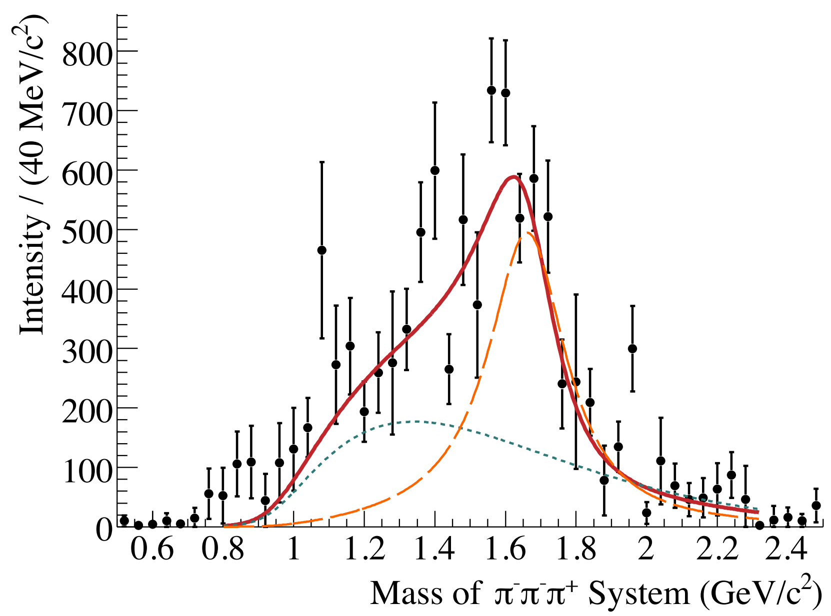
PRD83 111502 (2011)
PRD88 094595 (2013)

Exotic hybrid mesons in QCD?

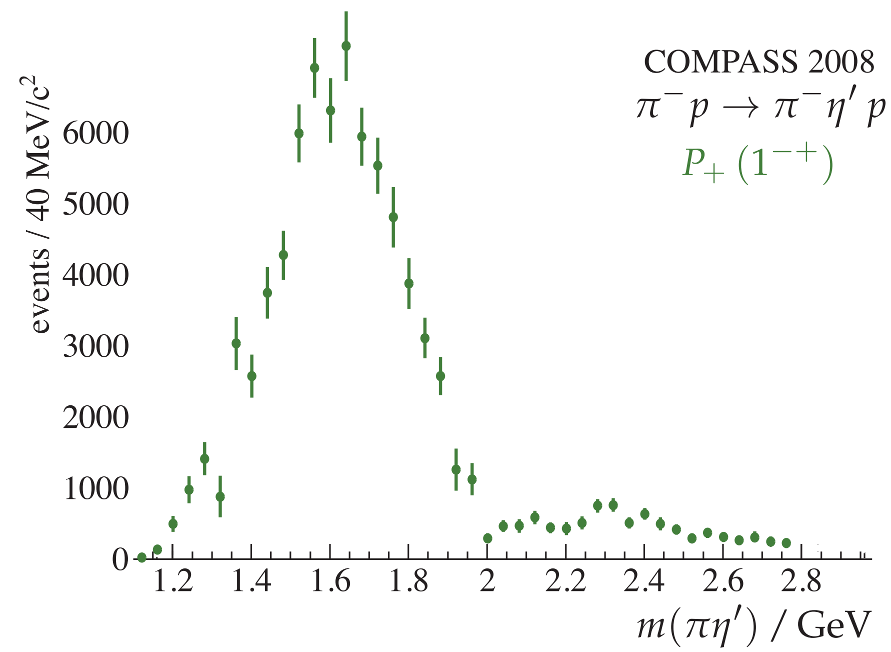
Excited states are resonances in scattering of lighter hadrons

We should see this in LQCD

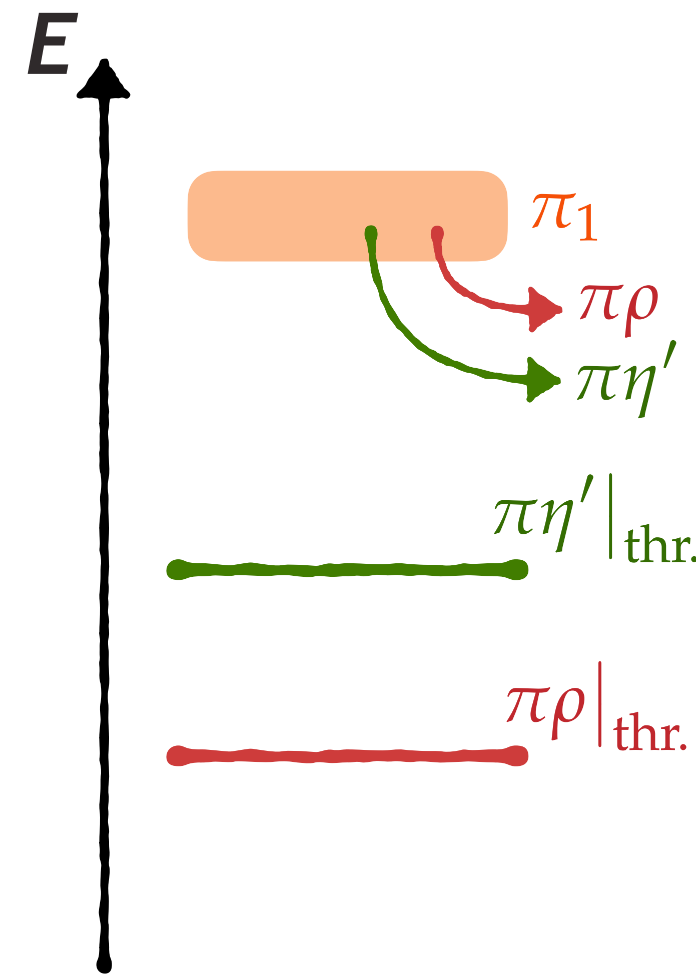
$1^{-+}\ [\rho\pi]_P$



$1^{-+}\ [\eta'\pi]_P$

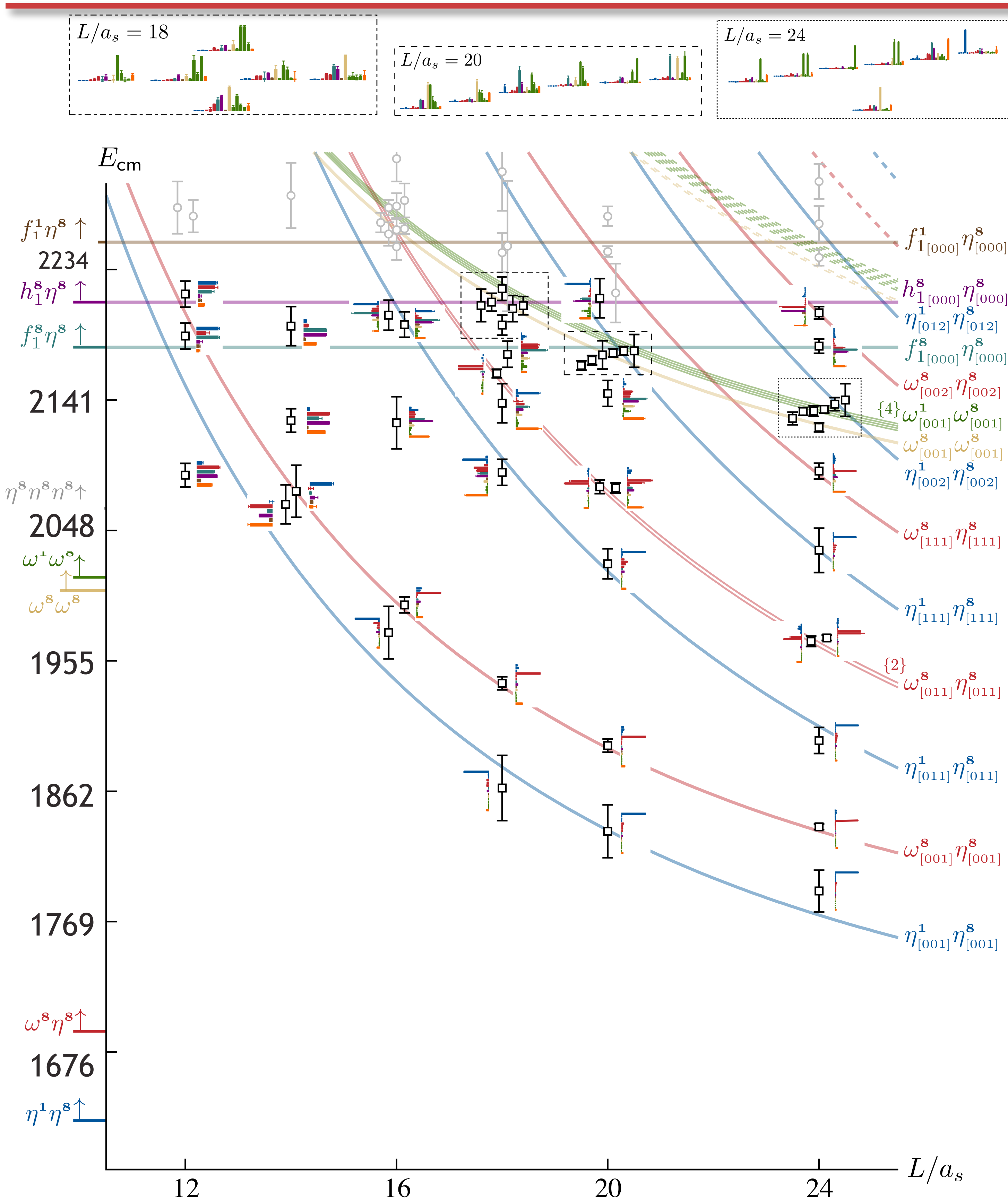


COMPASS Pb data
PRL104 241803 (2010)



Hard - but can change quark mass

Finite volume spectrum for exotic π_1



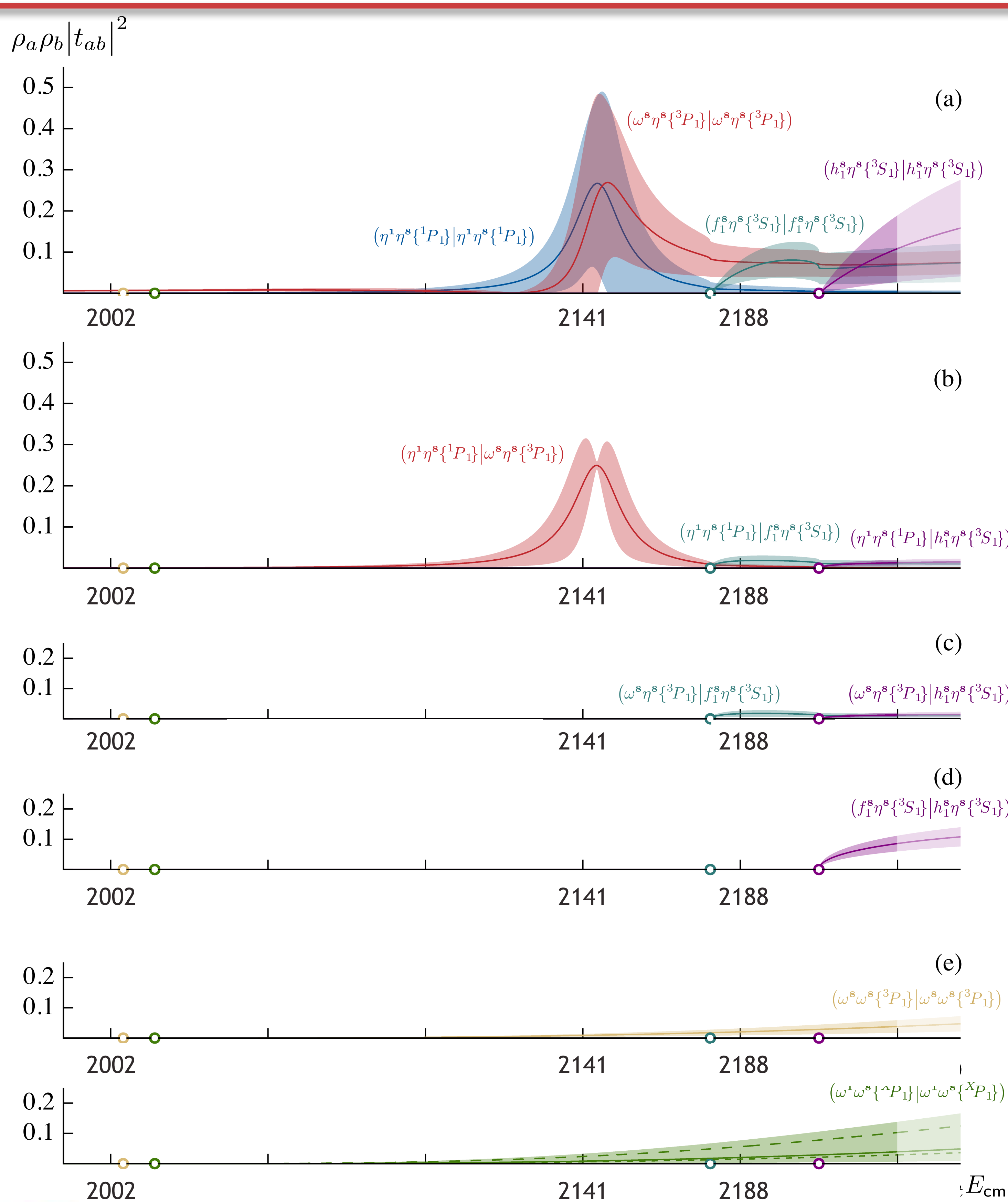
[Woss, et.al., Phys.Rev.D 103 (2021) 5, 054502]

"Scattering" formalism relates finite-volume energies to scattering amplitudes and hence resonances

Extract spectrum from extensive basis of operators - 63 energy levels

Fit to 8 channel scattering amplitude…

$J^{PC} = 1^{-+}$ scattering amplitudes



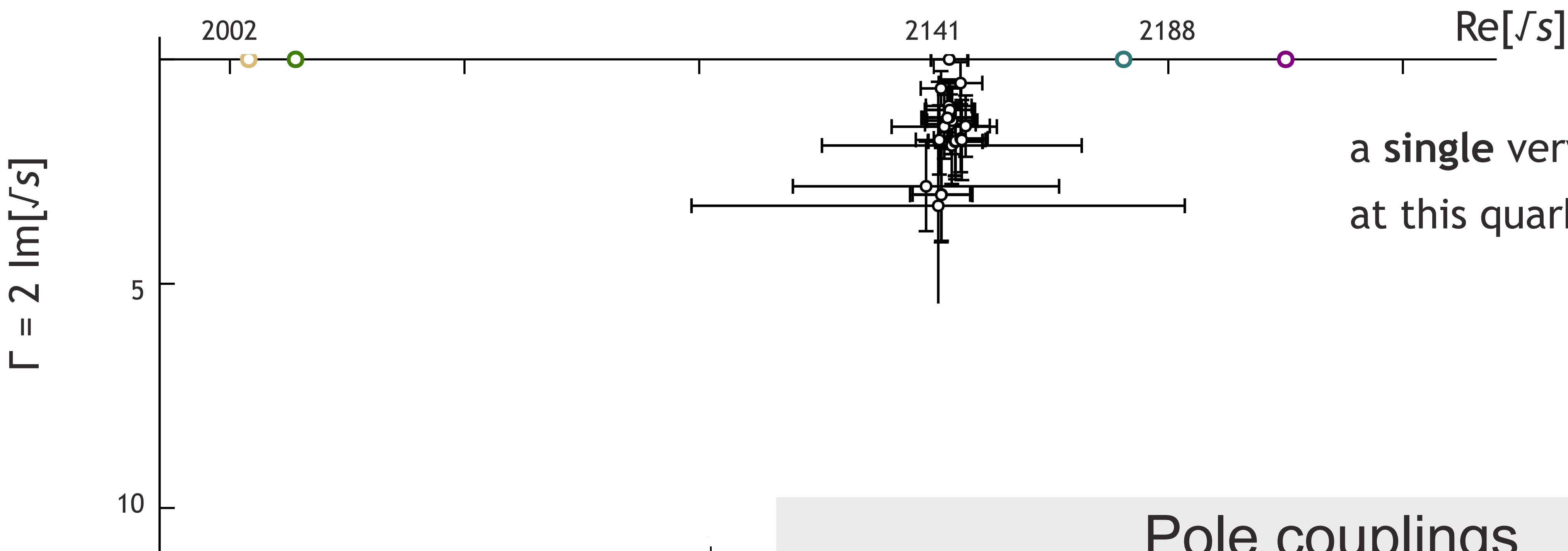
[Woss, et.al., Phys.Rev.D 103 (2021) 5, 054502]

diagonal elements
of scattering t-matrix

Scattering matrix - analytic function

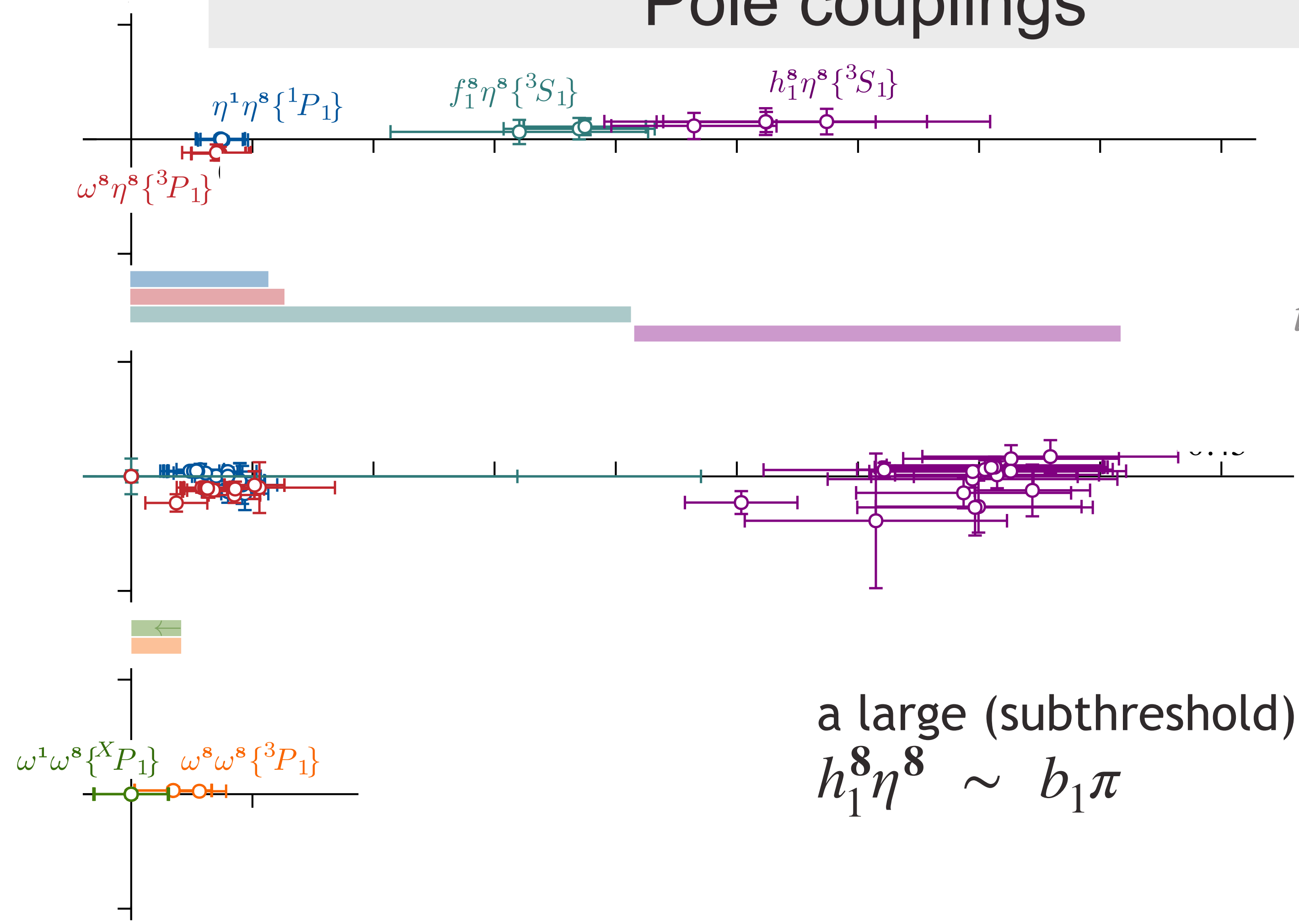
A resonant pole

[Woss, et.al., Phys.Rev.D 103 (2021) 5, 054502]



a **single** very narrow resonance at this quark mass

Pole couplings



$$t_{ab}(s) = \frac{c_a c_b}{s_0 - s}$$

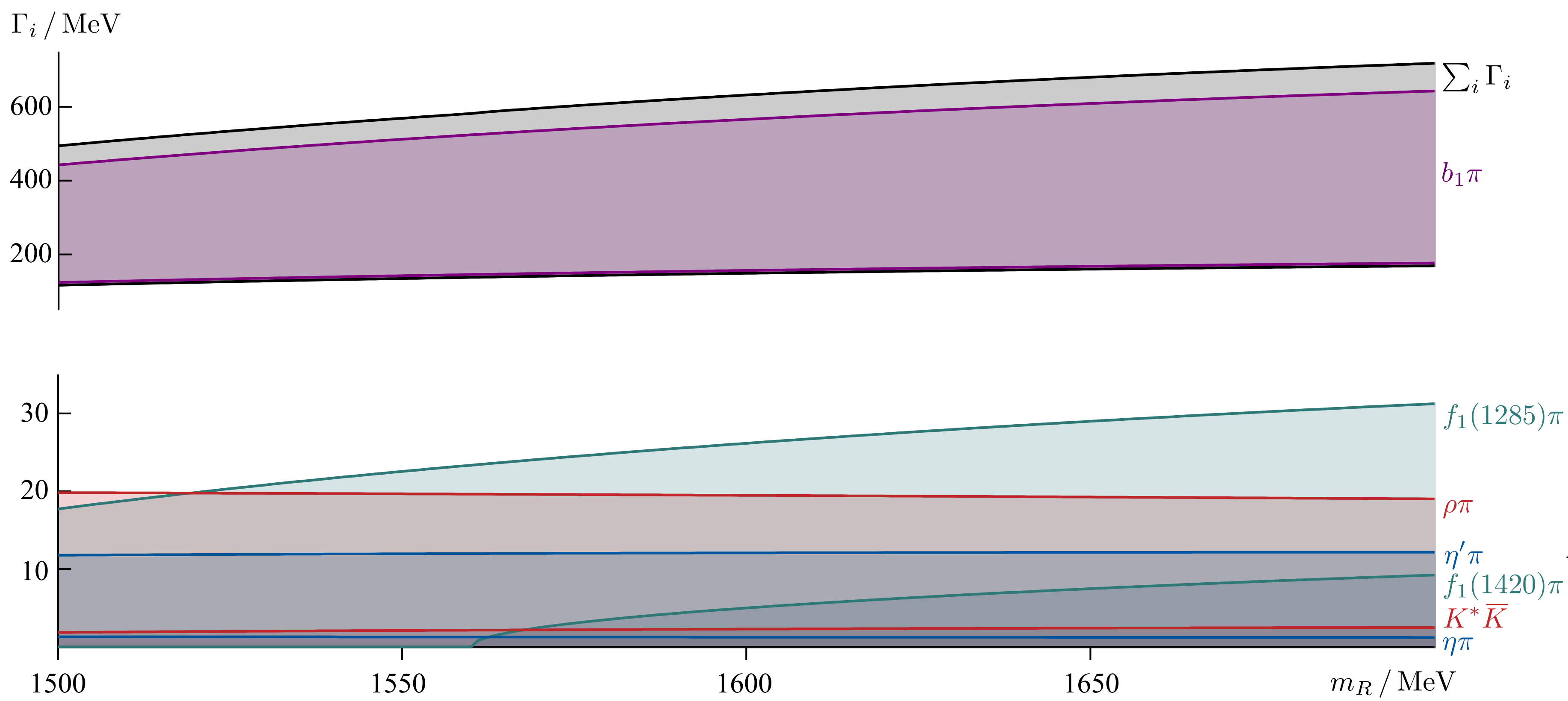
Couplings are directly comparable to expt.

a large (subthreshold) coupling to $h_1^{\mathbf{8}}\eta^{\mathbf{8}} \sim b_1\pi$

A prediction for exotic π_1 decay modes

Woss, et.al., Phys.Rev.D 103 (2021) 5, 054502

- First ever calculation - from QCD (quarks/gluons) - of full decay modes of an exotic
- **Major step forward for project**



$b_1\pi$ much larger than models suggest

GlueX searching here

- Expts looking in highly suppressed channels
- Results suggest exotic are broad resonances, but can be found in expt. (GlueX)

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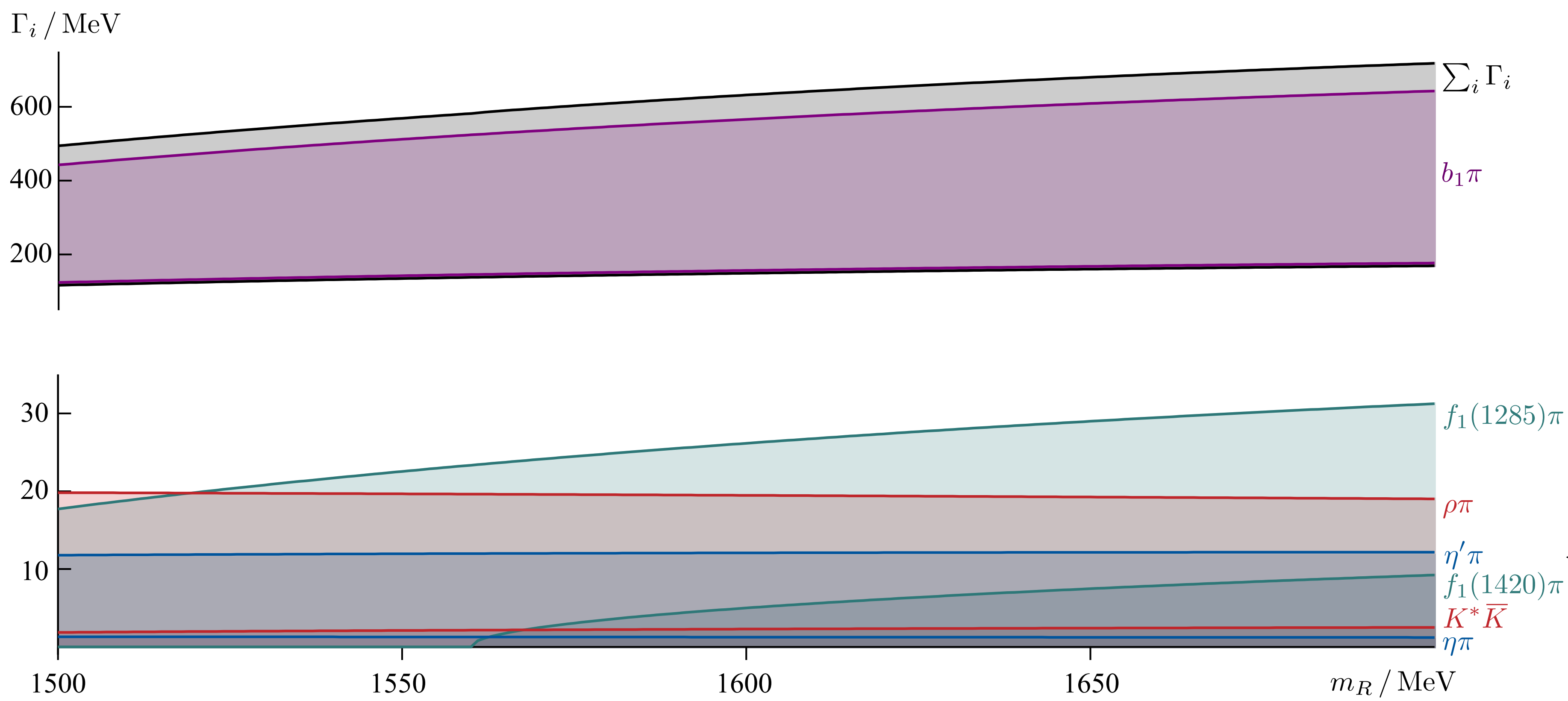

$b_1\pi$ much larger than models suggest

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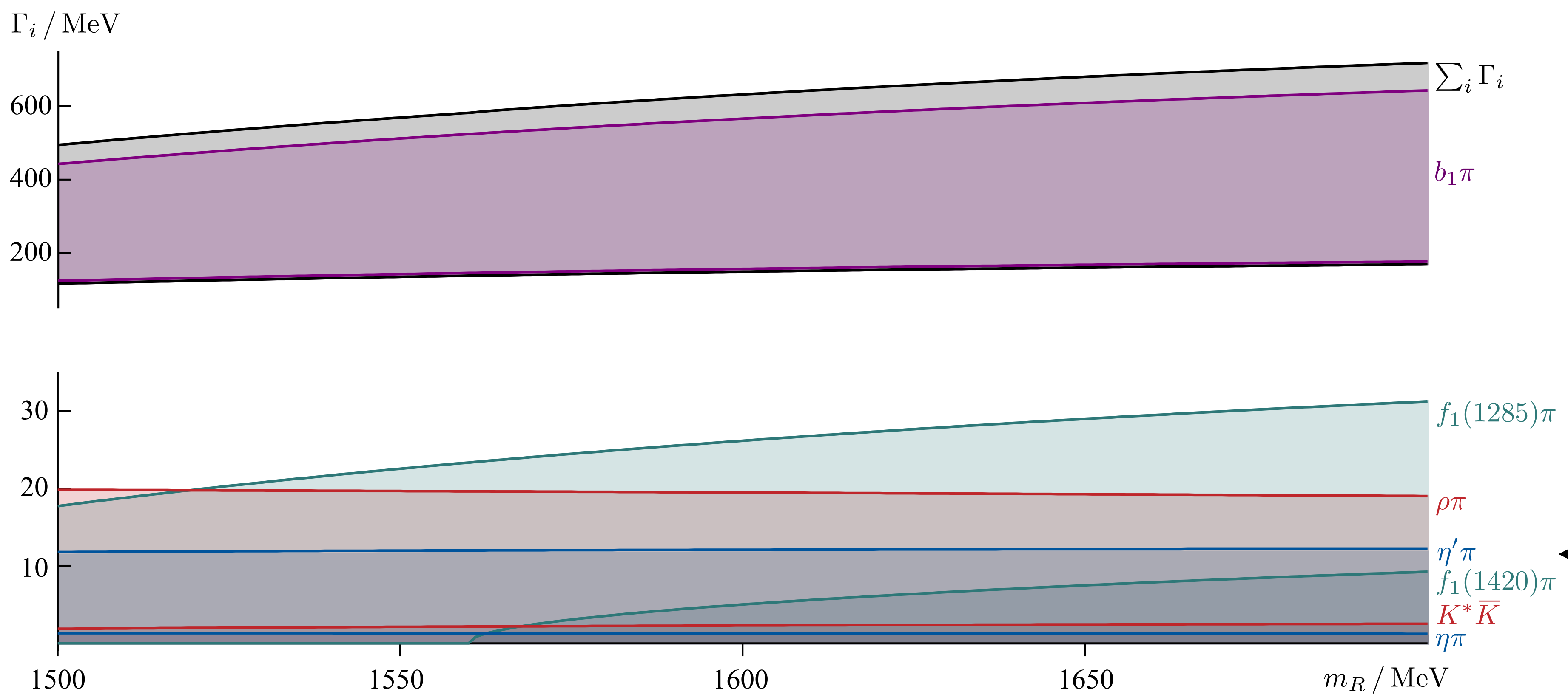
Steps forward - experiments looking for multiplets

A prediction for exotic π_1 decay modes

Woss, et.al., Phys.Rev.D 103 (2021) 5, 054502

- First ever calculation - from QCD (quarks/gluons) - of full decay modes of an exotic
- **Major step forward for project**



$b_1\pi$ much larger than models suggest

GlueX searching here

- Expts looking in highly suppressed channels
- Results suggest exotic are broad resonances, but can be found in expt. (GlueX)

Steps forward - experiments looking for multiplets

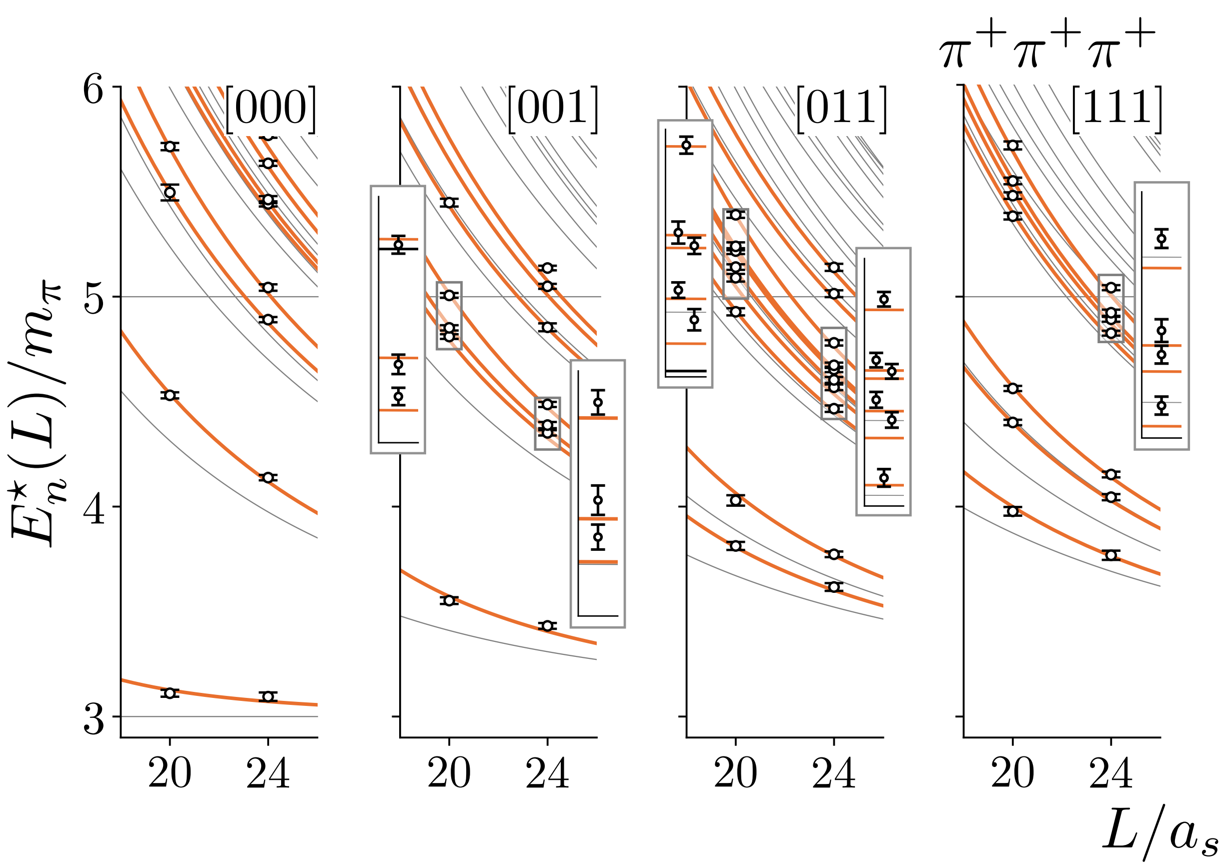
Can go beyond expts - investigate internal structure (gluonic pressure…)

Higher energies - first foray into 3-body decays

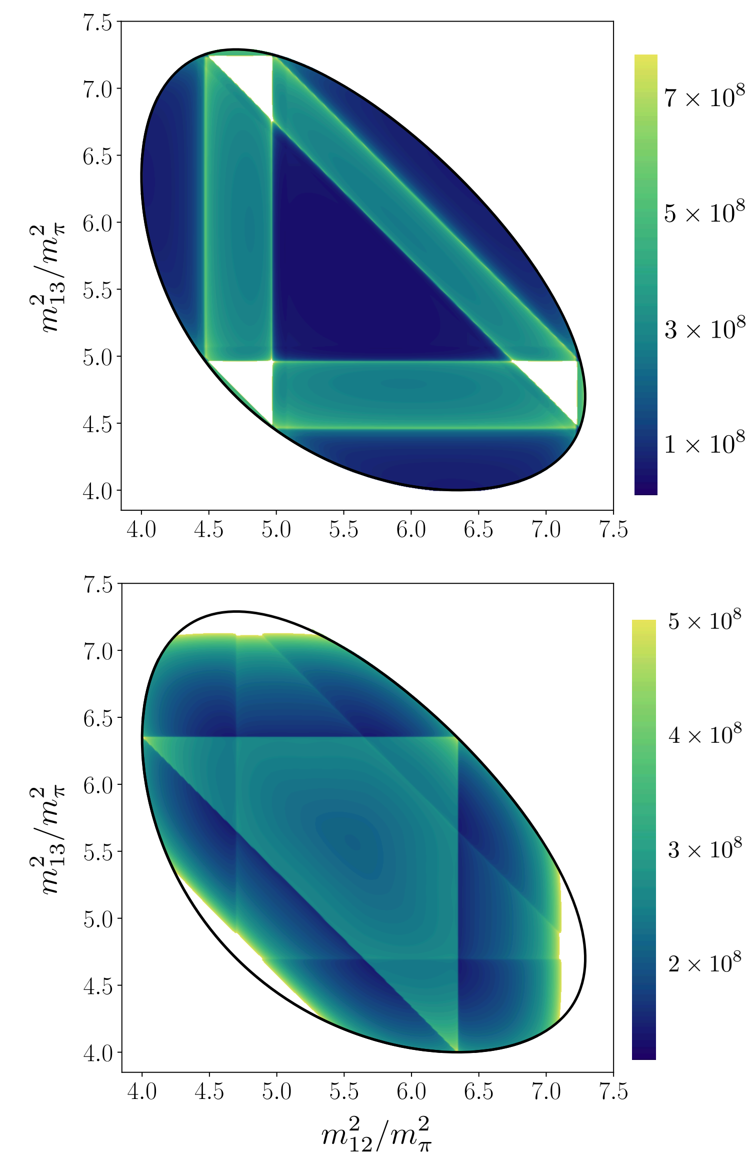
- Higher energy, need 3-body decays
- More complicated formalism
- First calculation of a 3-body amplitude
  - Computational challenge - more quarks/more graphs
  - Optimization of graph evaluation essential

Editor's Suggestion:

[Hansen, et.al., Phys.Rev.Lett. 126 (2021) 012001](https://doi.org/10.1103/PhysRevLett.126.012001)



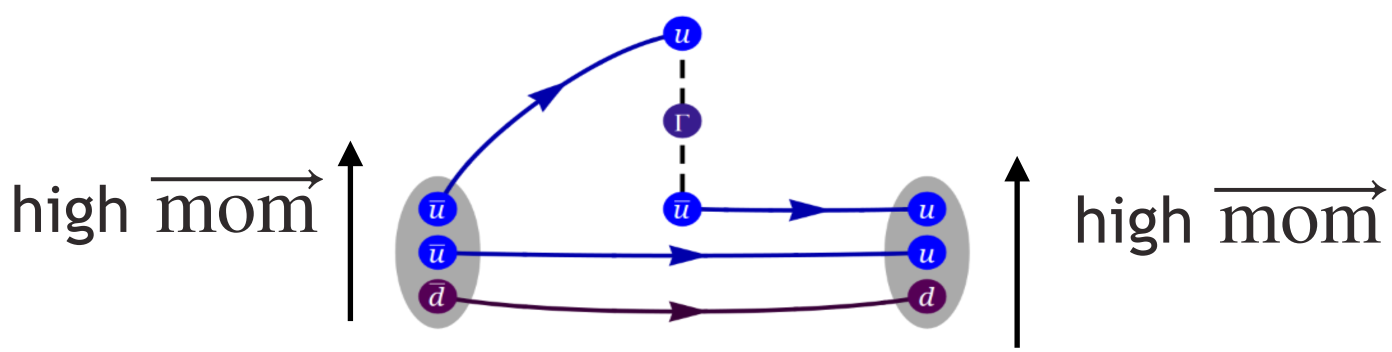
"Dalitz" plot - relation of energy pairs

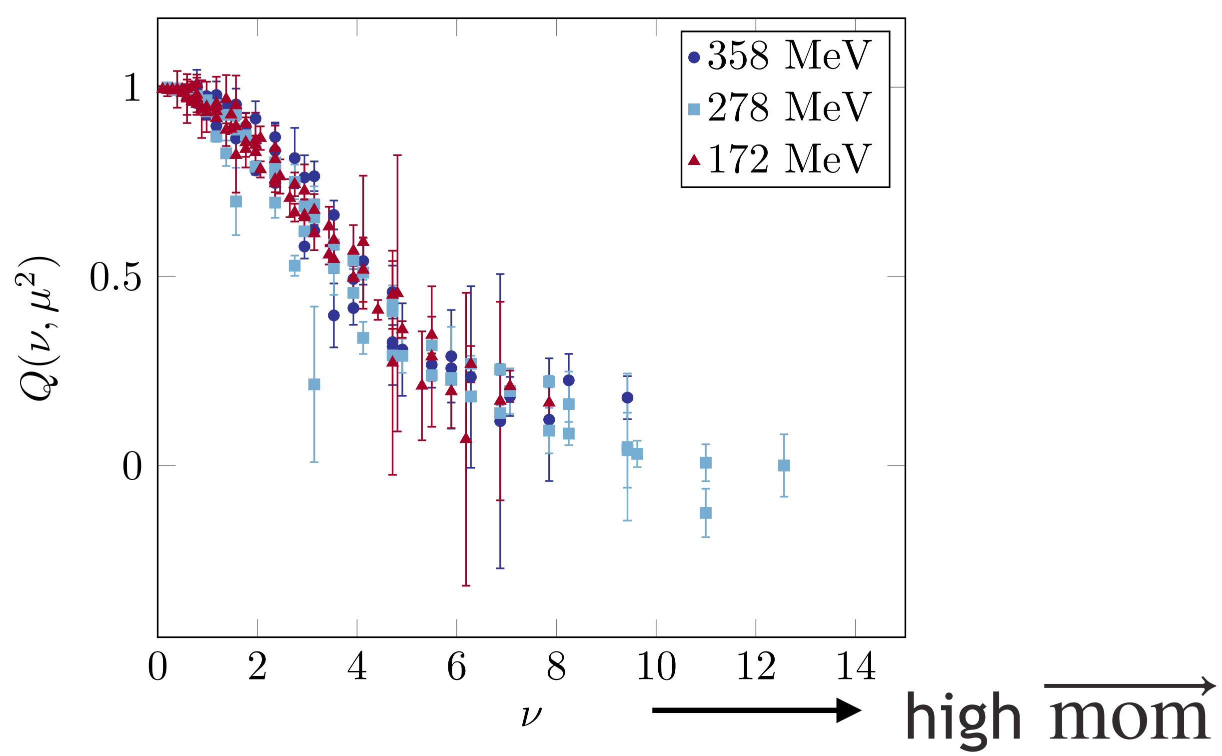


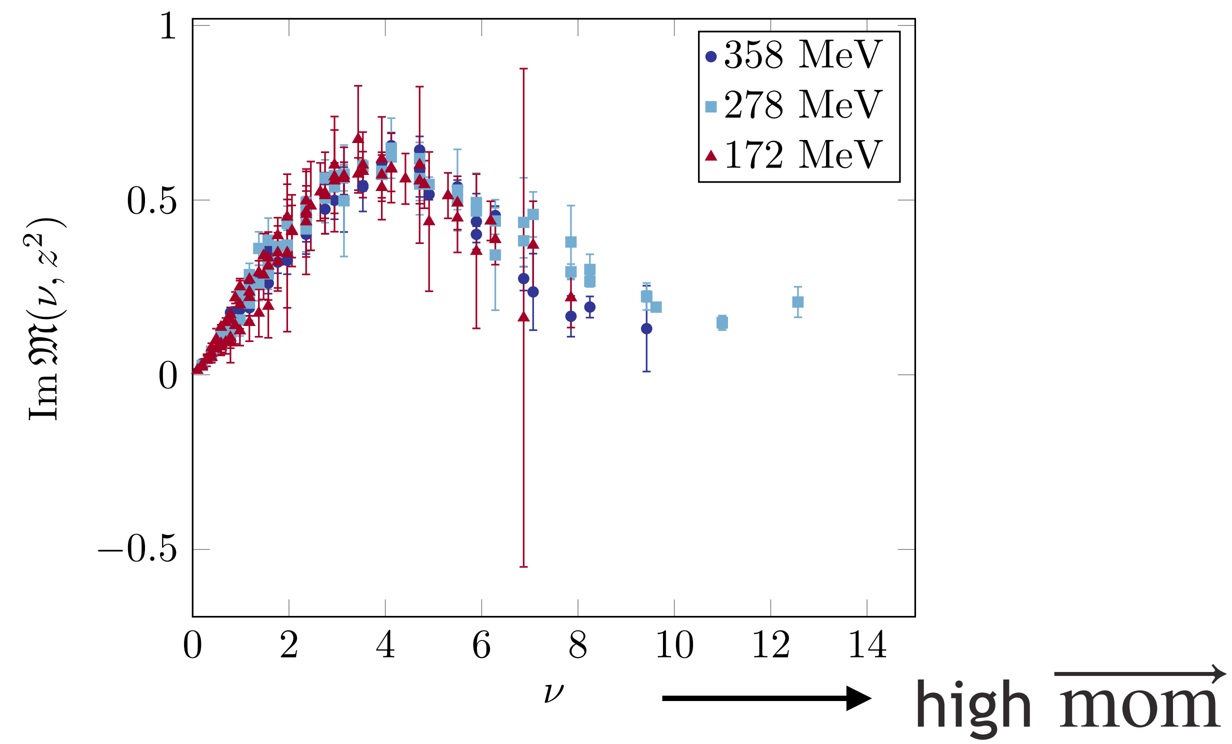
Jefferson Lab

Nucleon Parton Distribution Functions

- Key indicator of nucleon structure - measures arrangement of quarks in nucleon
- Any improvement benefits LHC searches. Focus of JLab12/RHIC & EIC
- Explosion of numerical & theoretical work ⇐ first USQCD studies.
    - Computational challenge - “insertions” w particles at high momentum (statistically noisy)
    - New algorithms!



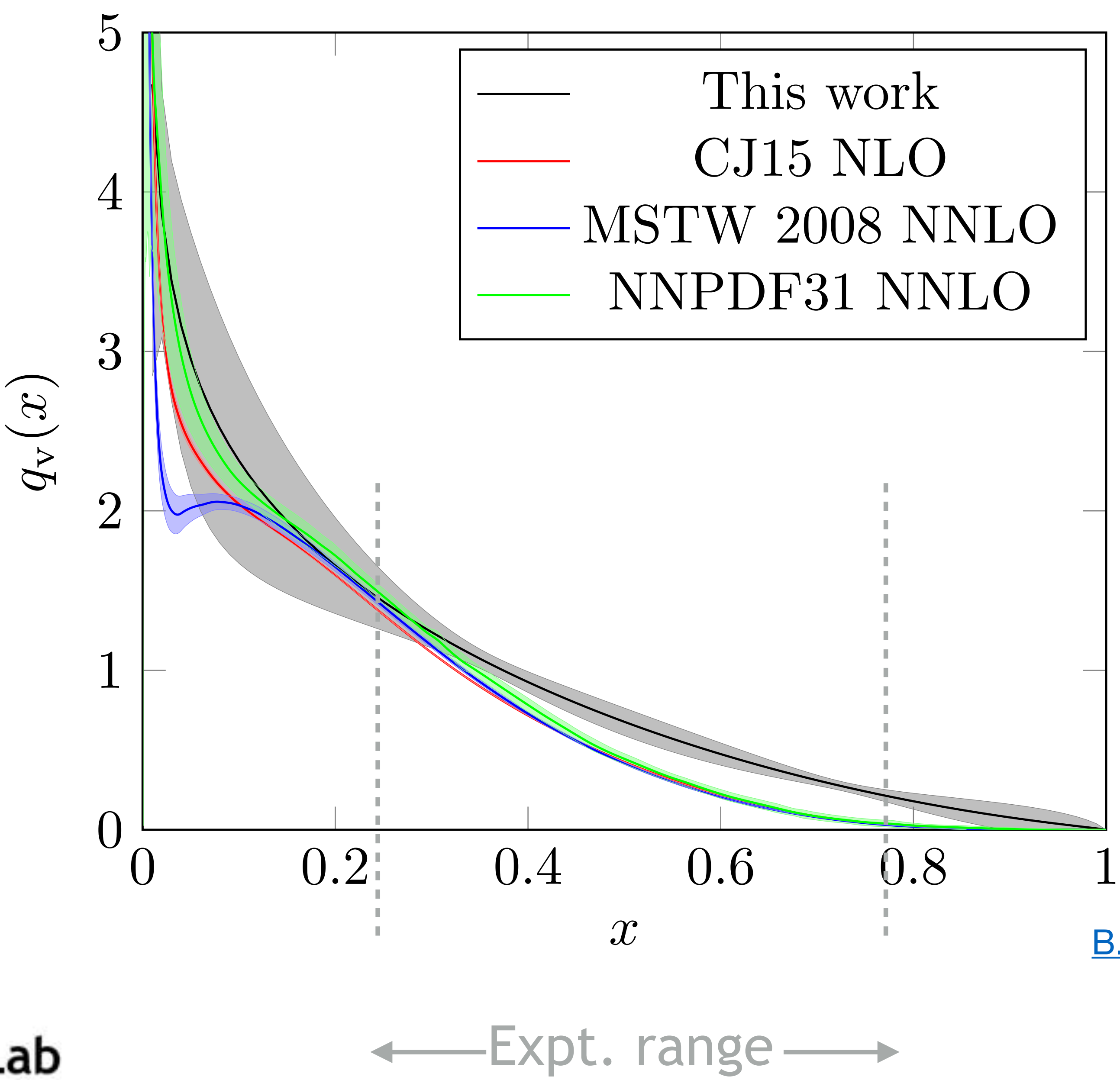




B. Joo et al., Phys.Rev.Lett 125, 232003 (2020)

Nucleon Parton Distribution Functions

- Key indicator of nucleon structure - measures arrangement of quarks in nucleon
- Explosion of numerical & theoretical work ⇐ first USQCD studies.
  - SciDAC essential - delivered on new algorithms



Expt./pheno methods limited by expt. data

Once thought unobtainable in LQCD

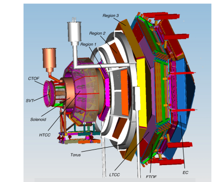
Demonstration of feasibility

Computing Generalized-PDF for JLab12

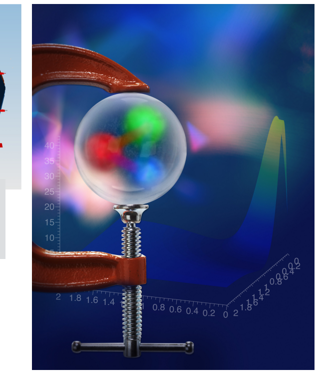
B. Joo et al., Phys.Rev.Lett 125, 232003 (2020)

Pressure in the proton

Pressure of quark/glue mapped in expt.

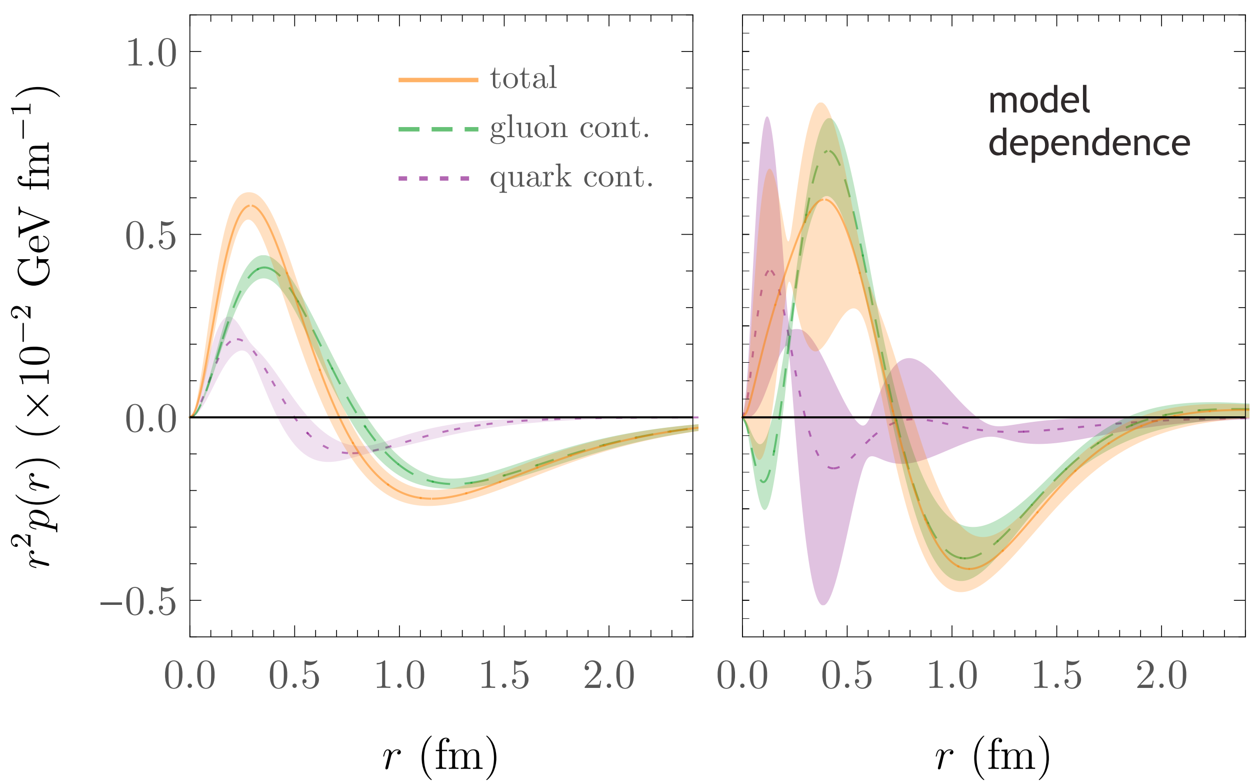


CLAS6

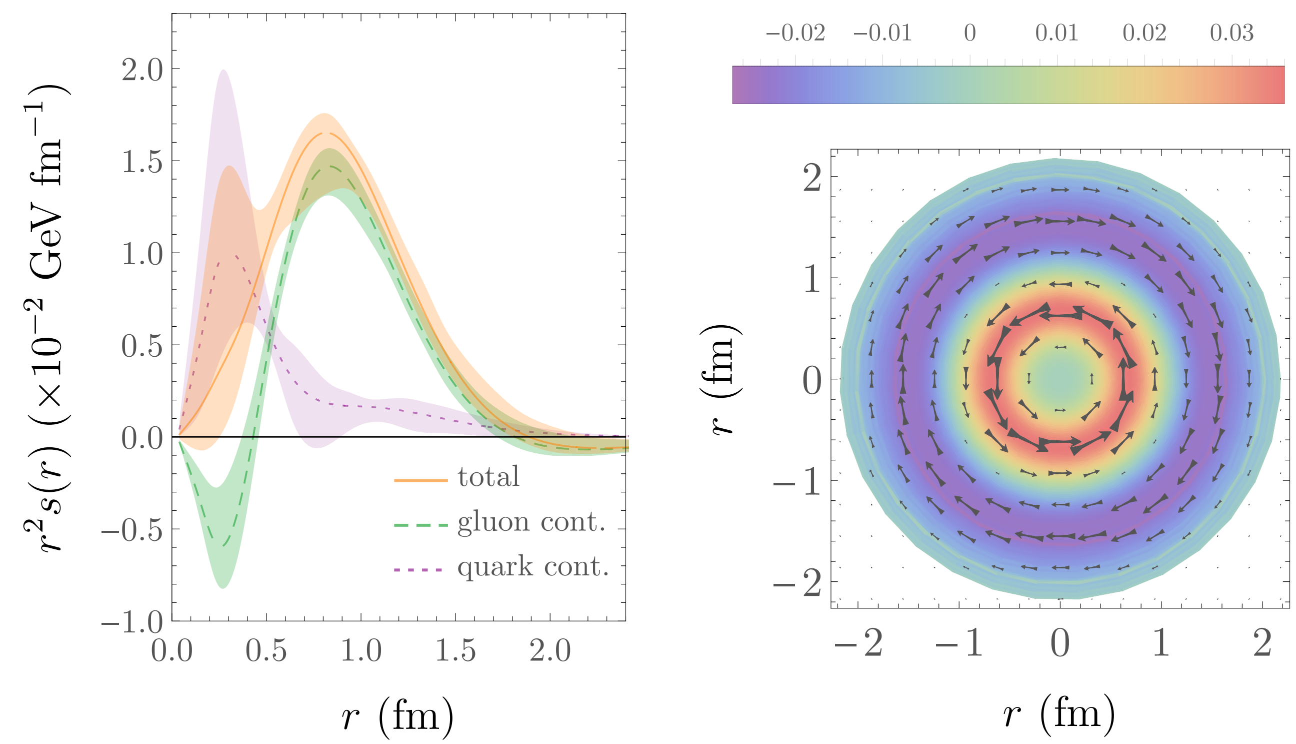


LQCD can compute Energy-Mom. Tensor matrix elements

r² * pressure



r² * shear



quarks/glue repulsive at core; attractive at boundary

glue lurks near boundary

PRL122, 072003 (2019)

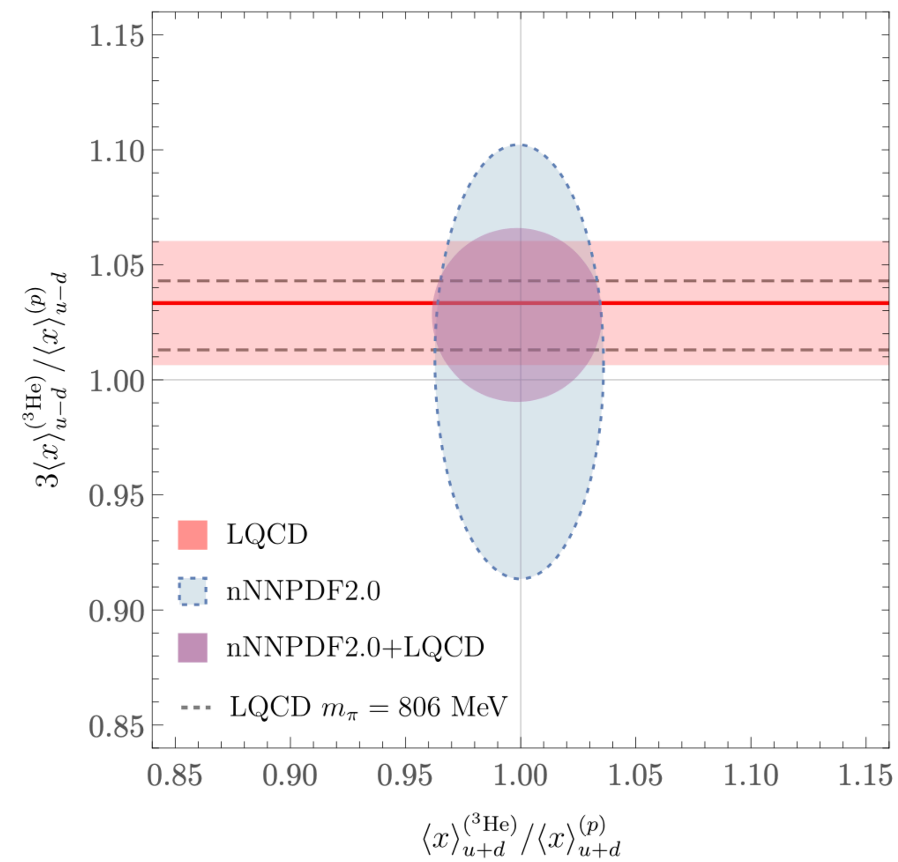
^{3}He Parton Distribution Functions

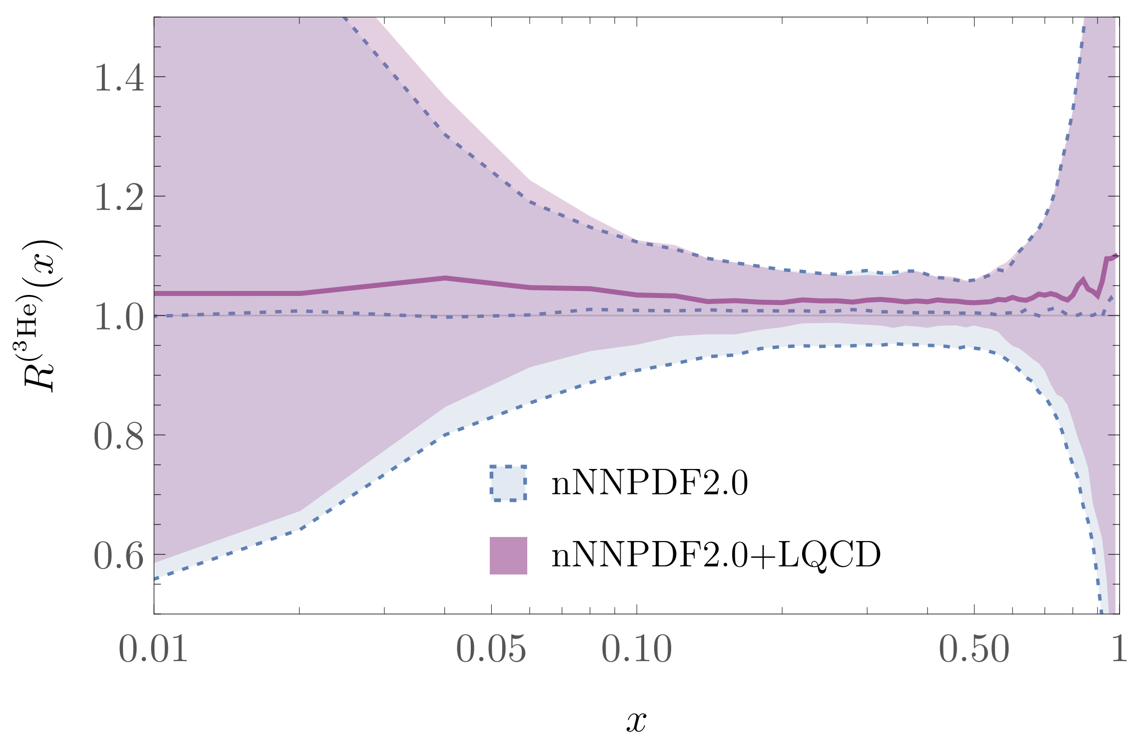
- Are nuclei just collections of nucleons?
- Poorly known experimentally
- First study in nuclei - albeit large pion mass
  - Computational challenge - nuclear many-body wave functions computationally intensive
  - (See first examples from spectroscopy)

Detmold, et al., arXiv:2009.05522, submitted to PRL

^{3}He Parton Distribution Functions

- Are nuclei just collections of nucleons?
- Poorly known experimentally
- First study in nuclei - albeit large pion mass
    - Single moment in ^{3}He very close to proton
    - Combining with phenomenological reduces uncertainties ~2.5x
    - Door open to include techniques used for nucleons

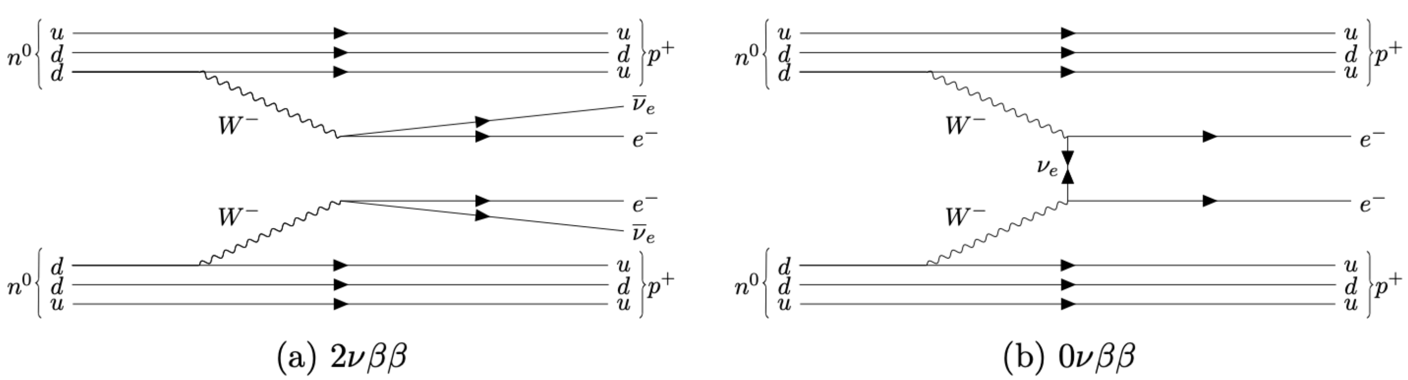




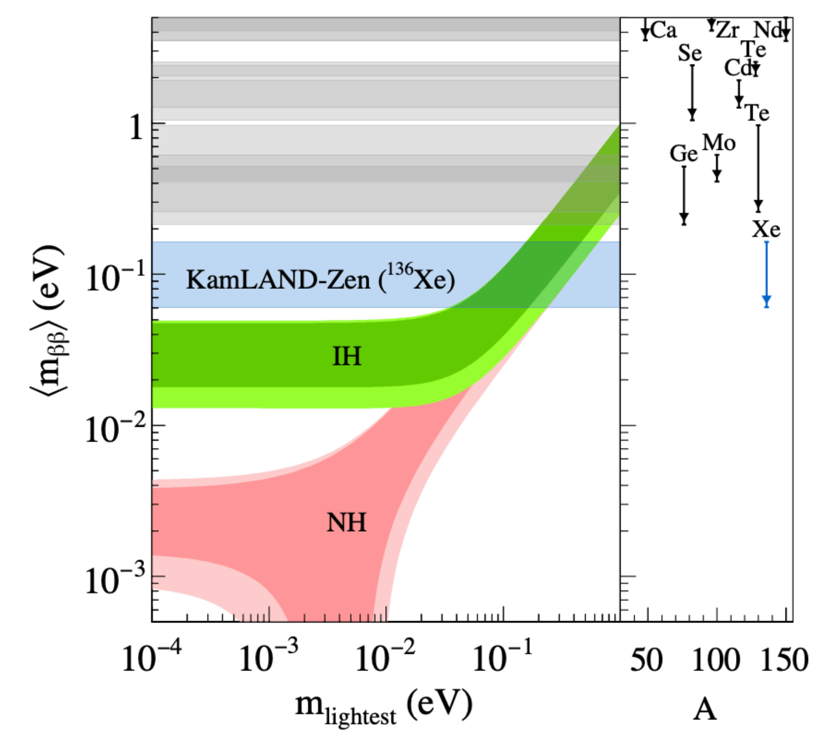
Detmold, et al., arXiv:2009.05522, submitted to PRL

Fundamental symmetries

- Low energy nuclei can serve as a sensitive probe of beyond Standard-Model physics
- Focus of Fundamental Symmetries program of DOE & expt
  - Computational challenge - nuclear many-body wave functions
  - Long-range matrix elements - computationally expensive in propagators



Neutrino-ful and -less decays
Manifested as matrix elements of QCD processes



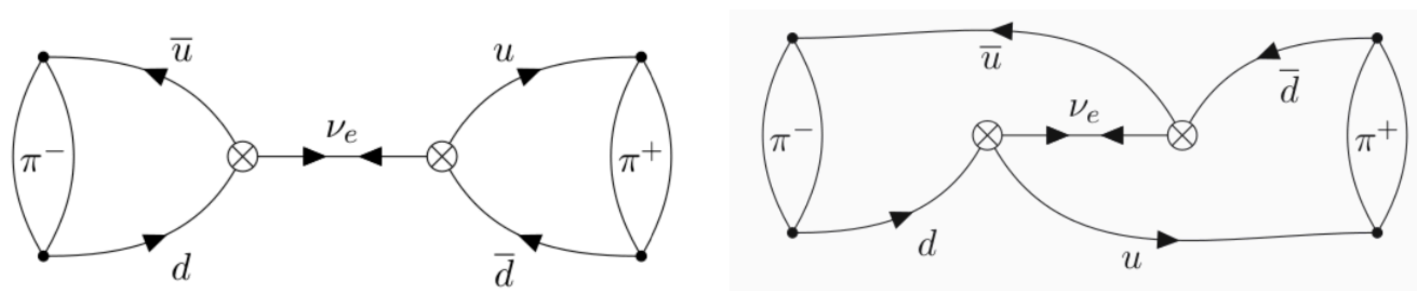
Larger nuclei more sensitive

Hard! - first establish formalism

Detmold, et al., arXiv:2004.07404, submitted to PRL

Fundamental symmetries

- Low energy nuclei can serve as a sensitive probe of beyond Standard-Model physics
- Focus of Fundamental Symmetries program of DOE & expt
  - First tests in simplified system - within a π
  - Future tests confront nuclei systems



(b) Type (1) contraction (c) Type (2) contraction

Comparable results in different methods - validating formalism

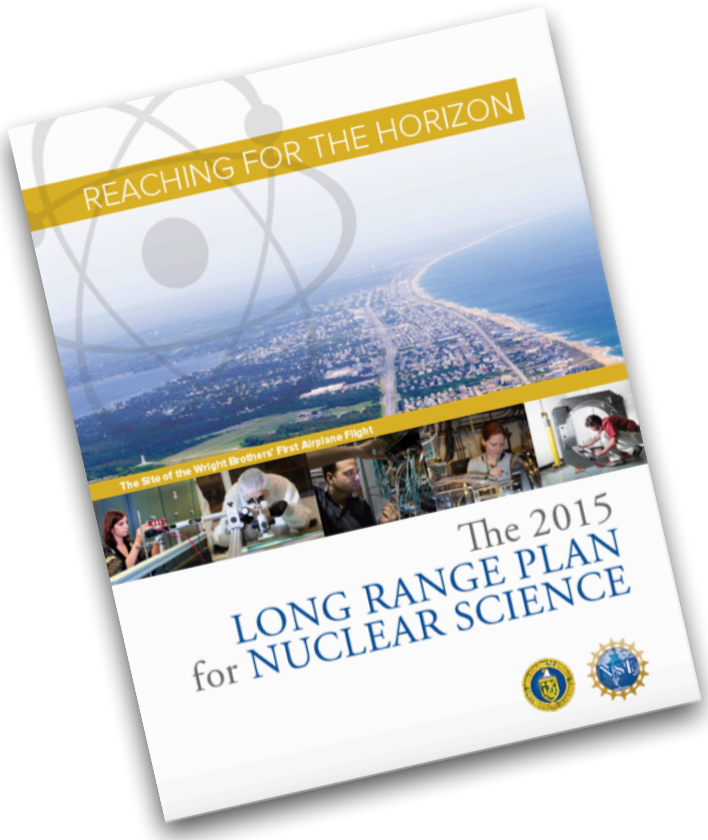
$$
\begin{aligned}
g_\nu^{\pi\pi}(\mu = 770\ \mathrm{MeV}) &= -11.96(31), && (\pi^-\pi^- \to e^-e^-) \\
&= -10.89(28)(33)_L(66)_a, && (\pi^- \to \pi^+ e^- e^-) \\
&= -10.78(12)(51), && (\pi^- \to \pi^+ e^- e^-)
\end{aligned}
$$

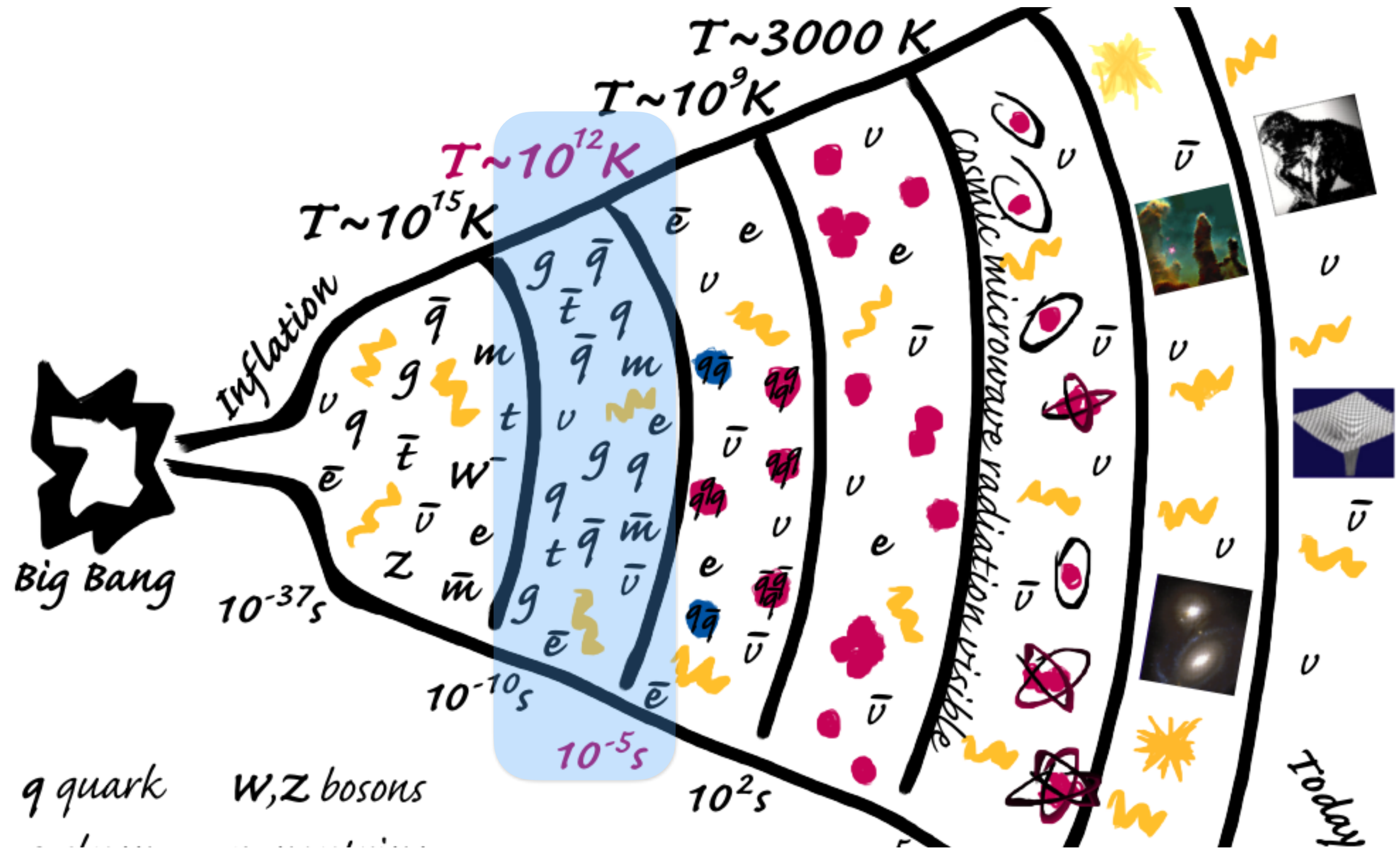
Detmold, et al., arXiv:2004.07404, submitted to PRL

Hot-Dense matter

properties of quark gluon plasma (QGP)

the big questions …



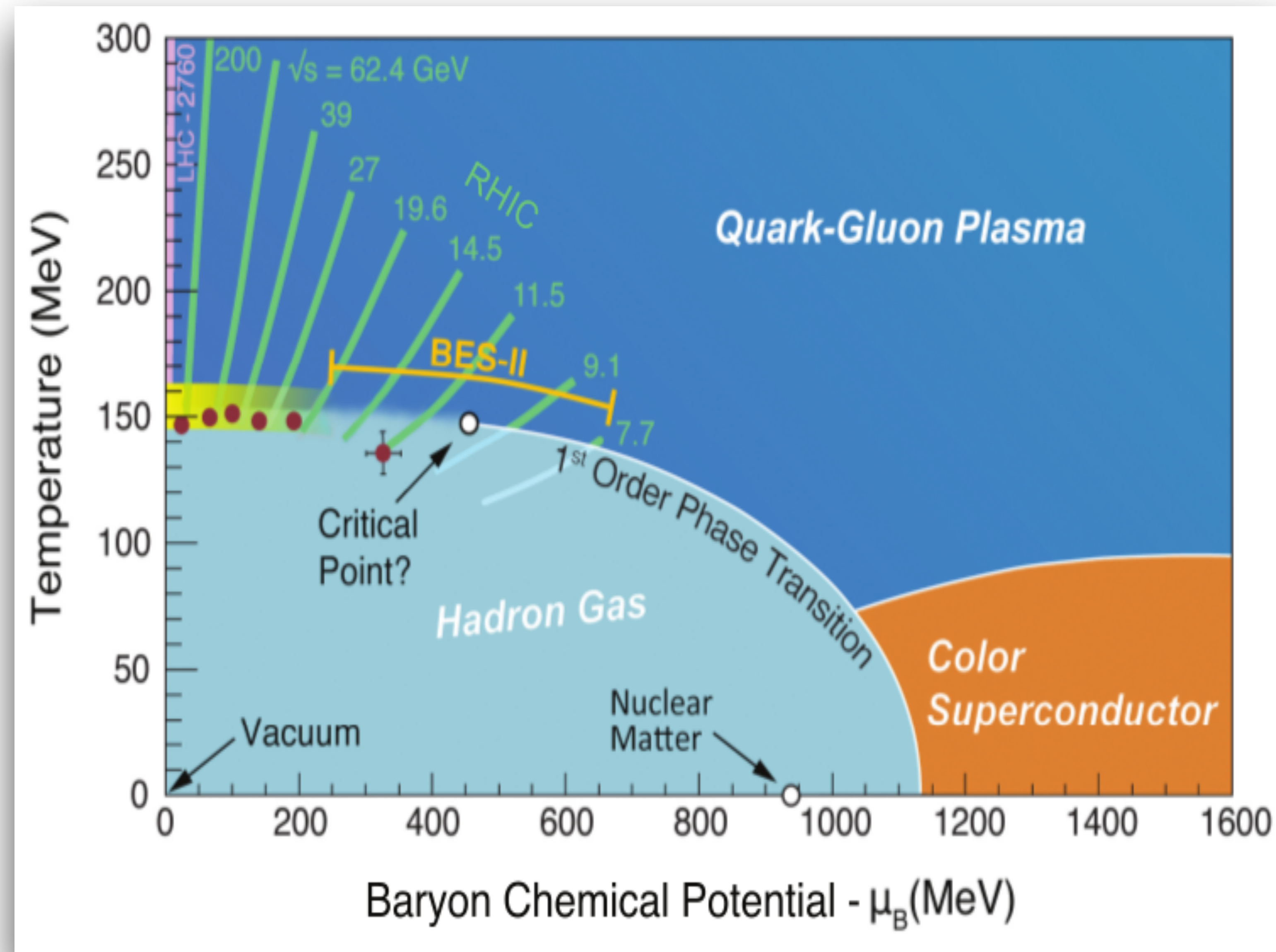


characterize the matter that existed
~ micro-seconds after the Big Bang

Hot-Dense matter

properties of strongly interacting matter

the big questions ...



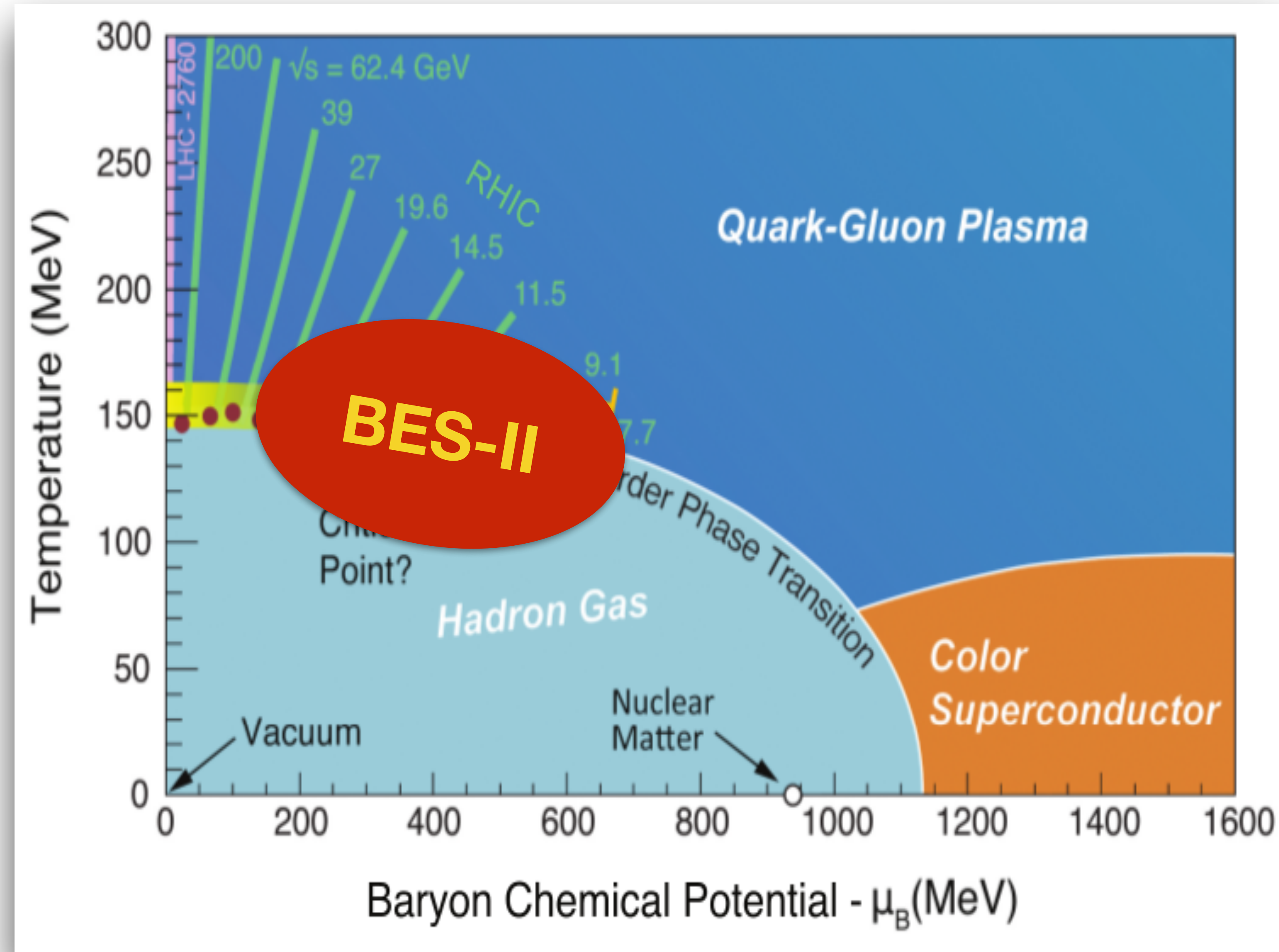
- varying temperatures and densities

Hot-Dense matter - new expt. at BNL

Beam Energy Scan-II @ RHIC

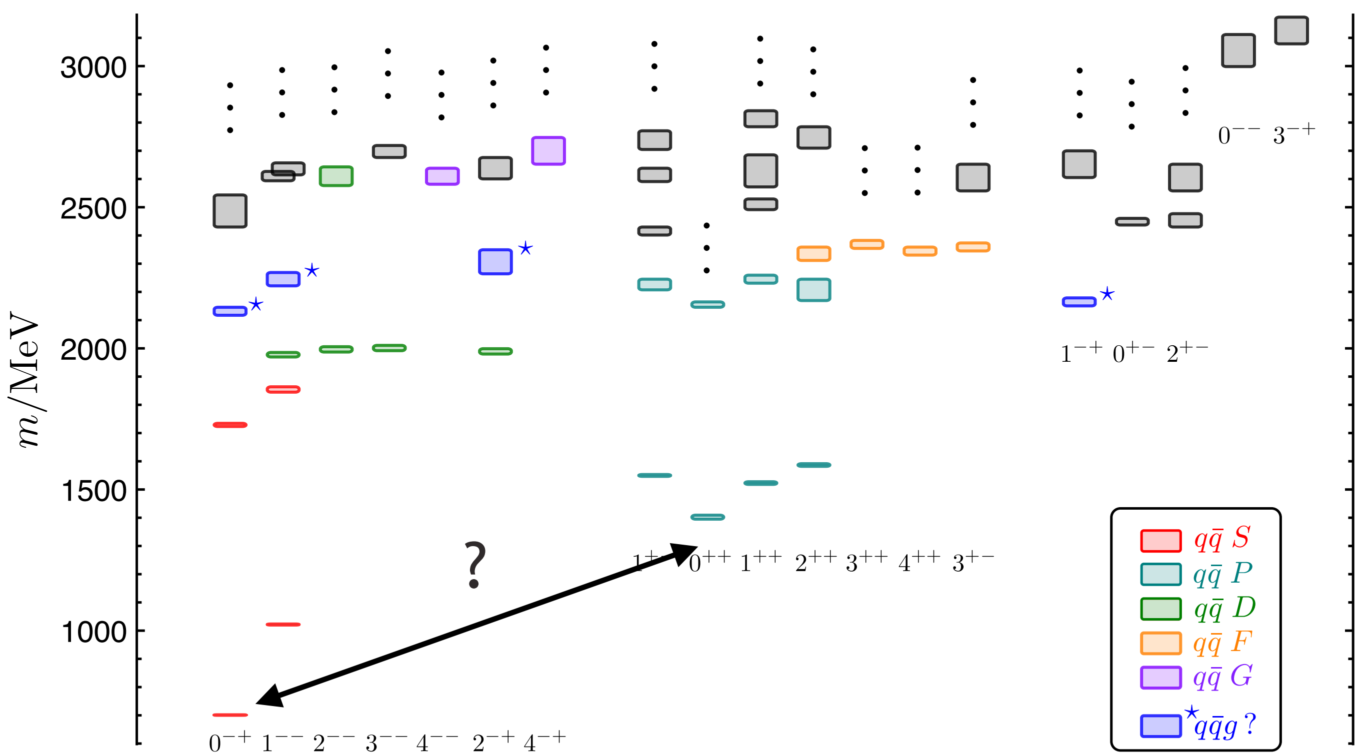
2019-2021

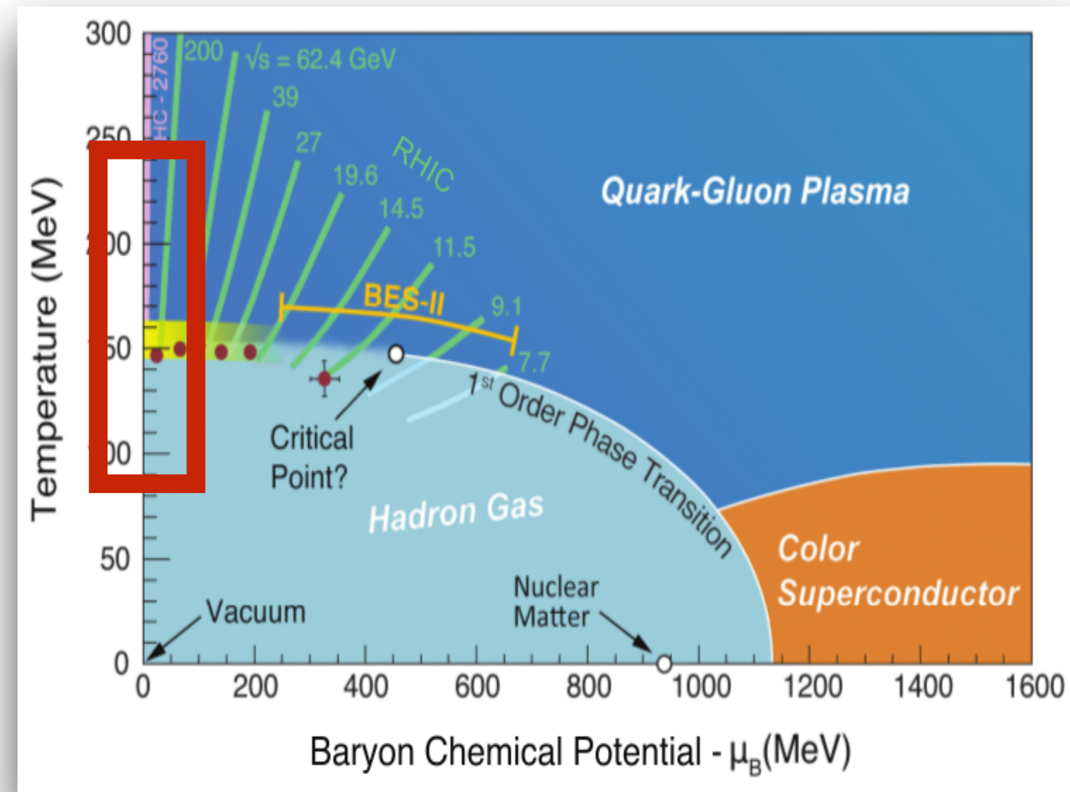
Phase diagram? Critical point?



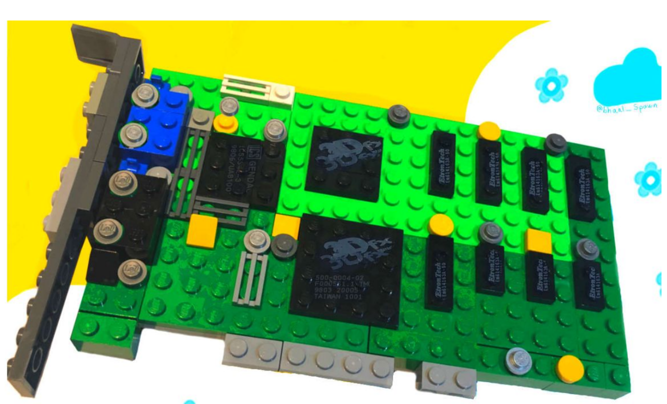
Temperature and mass generation

- Thought topological modes gives rise to breaking of chiral symmetry & hence mass
  - (HadSpec!) Spectroscopy calculations give nonzero mass splitting of π-a_0, and η-f_0
  - Is this maintained at non-zero temperature?





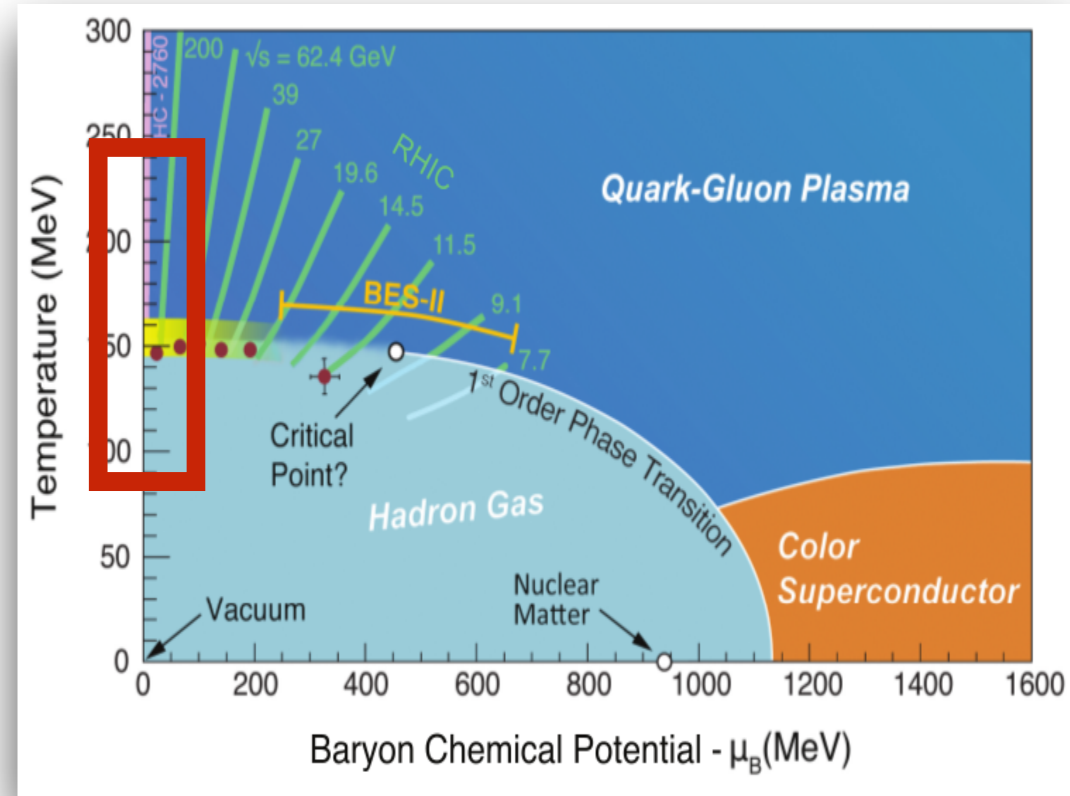
- Computational challenge - large number of Dirac inverses (linear systems of eqns.)
- GPU-s!

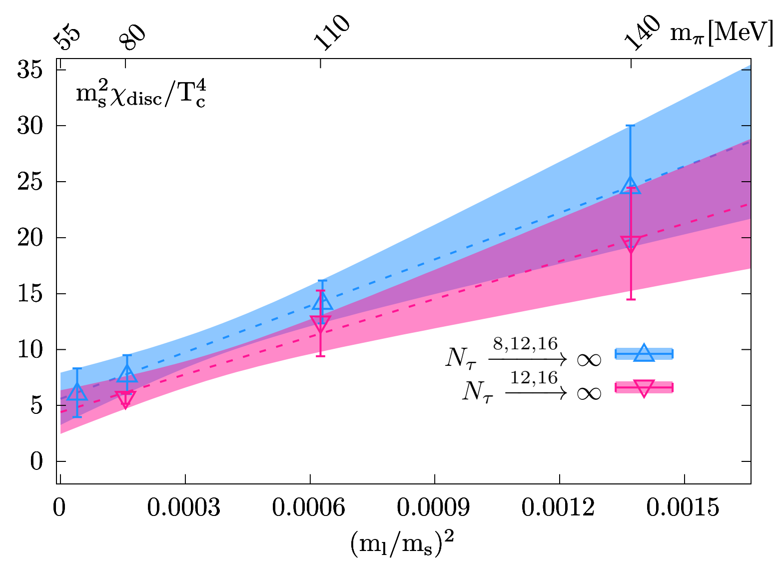


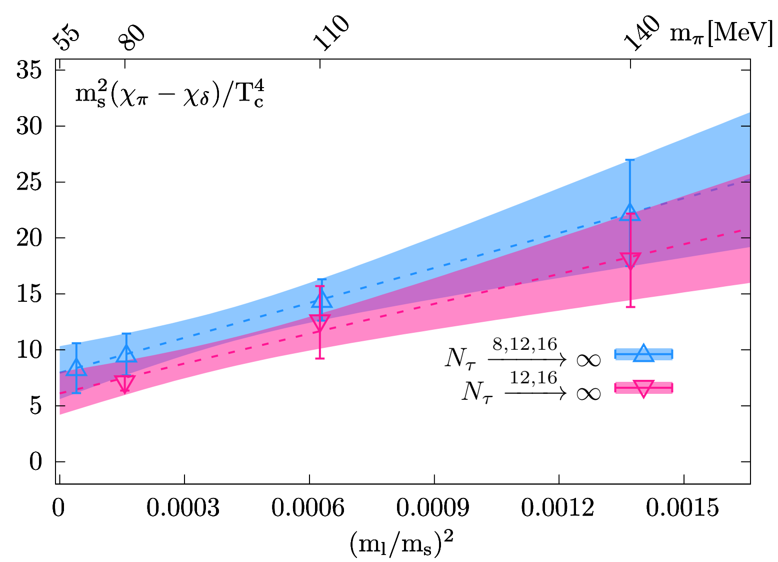
[H.T. Ding, et al., Phys.Rev.Lett 126 (2021) 8,082001]

Temperature and mass generation

- Thought topological modes gives rise to breaking of chiral symmetry & hence mass
  - YES - mass-splittings maintained at non-zero temperature
  - Nice connection amongst LQCD/SciDAC results







H.T. Ding, et al., Phys.Rev.Lett 126 (2021) 8,082001

LQCD workflow & computational requirements

Gauge generation
- Leadership level
- Strong scaling

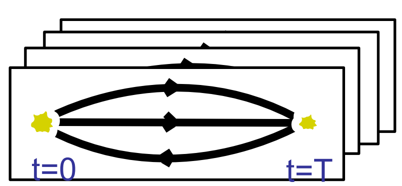
Strong scaling limited
- Comms/compute less balanced in recent machines
- Latency in comms important
- Require comms reduced linear solvers
- Sympletic PDE integrators
- Data-parallel code gen. with comms

Analysis
- Throughput level
- O(1M) RHS-s/cfg

Throughput challenge
- Solvers still important
- Large problems / node -> minimize memory traffic

Contractions

Correlators
- O(1M)/cfg

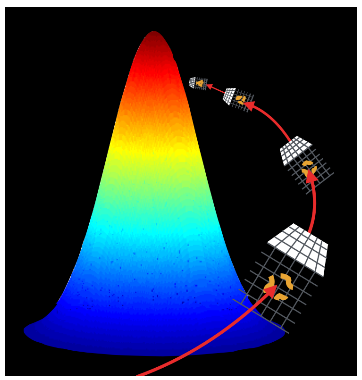


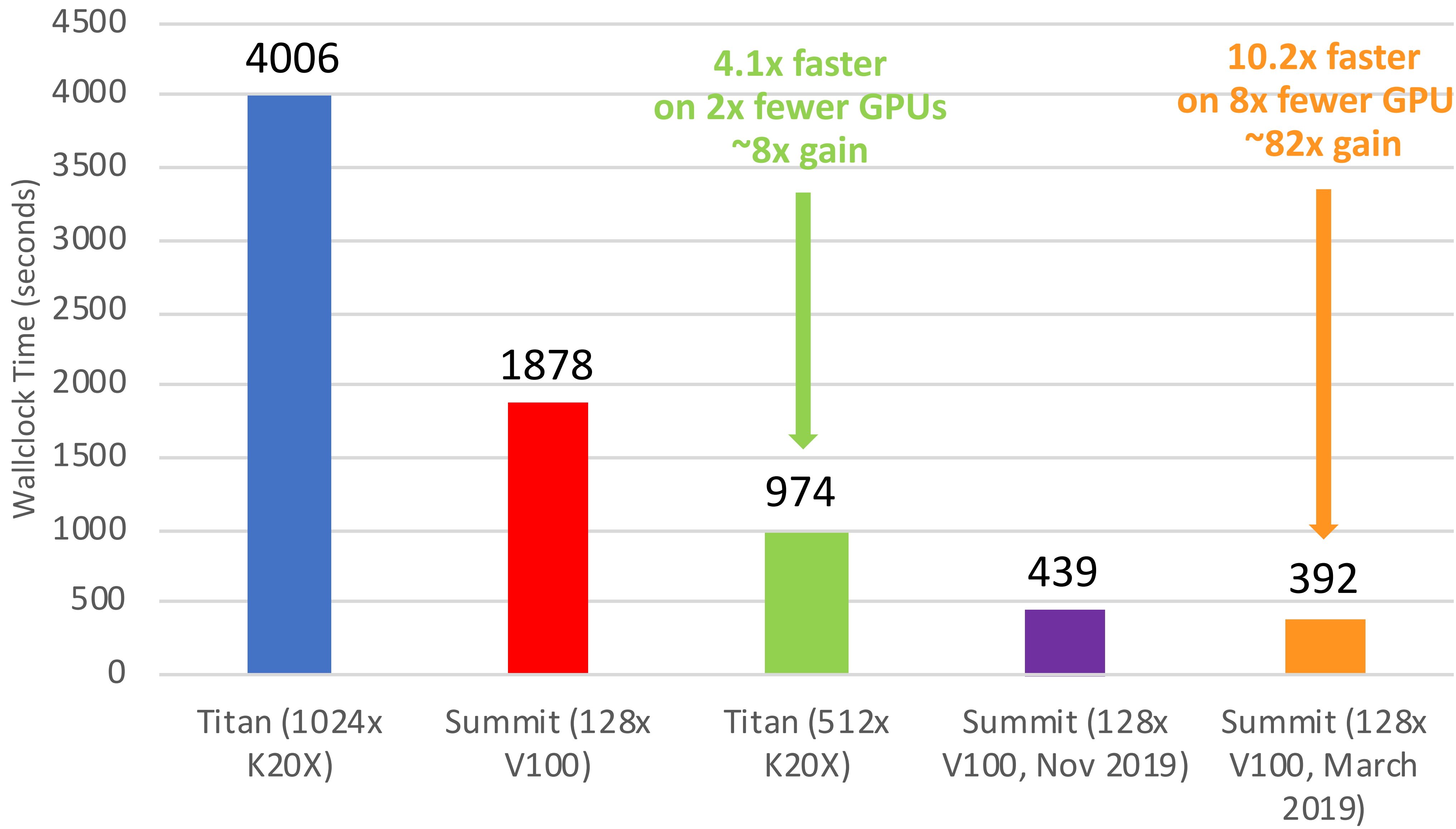
"Workflow" challenge
- Combinatorics -> improved graph theoretic methods
- Code generation for (sparse) tensor contractions
- Job coordination -> opportune for grid based

Accelerating QCD gauge generation on GPUs

Collaboration involving ASCR support and Industry partners

Chroma





- **~10.2x** wallclock speed-up on Summit using **8x** fewer GPUs than Titan: **~82x improvement in computational efficiency**
- **Allows previously unaffordable calculations**

Next: Improved “thoughput”

Gauge generation
- Leadership level
- Strong scaling

Strong scaling limited
- Comms/compute less balanced in recent machines
- Latency in comms important
- Require comms reduced linear solvers
- 1-flavor solvers

Sympletic PDE integrators

Data-parallel code gen. with comms

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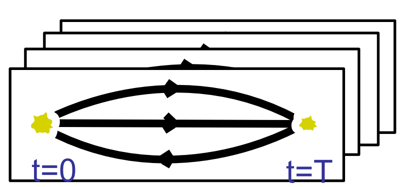
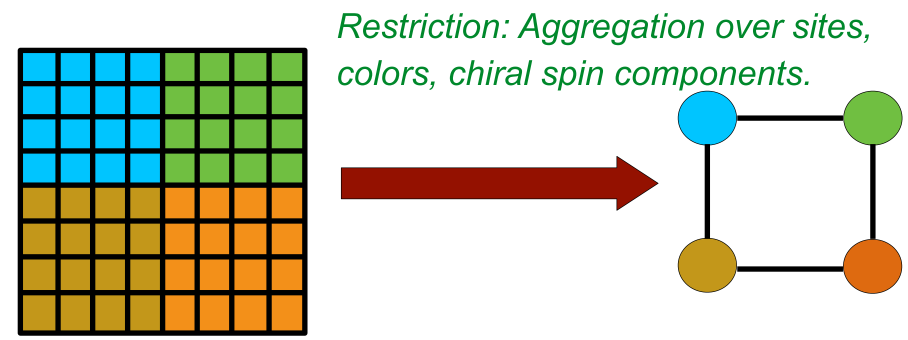


“Workflow” challenge
- Combinatorics -> improved graph theoretic methods
- Code generation for (sparse?) tensor contractions
- Job coordination -> Grid based

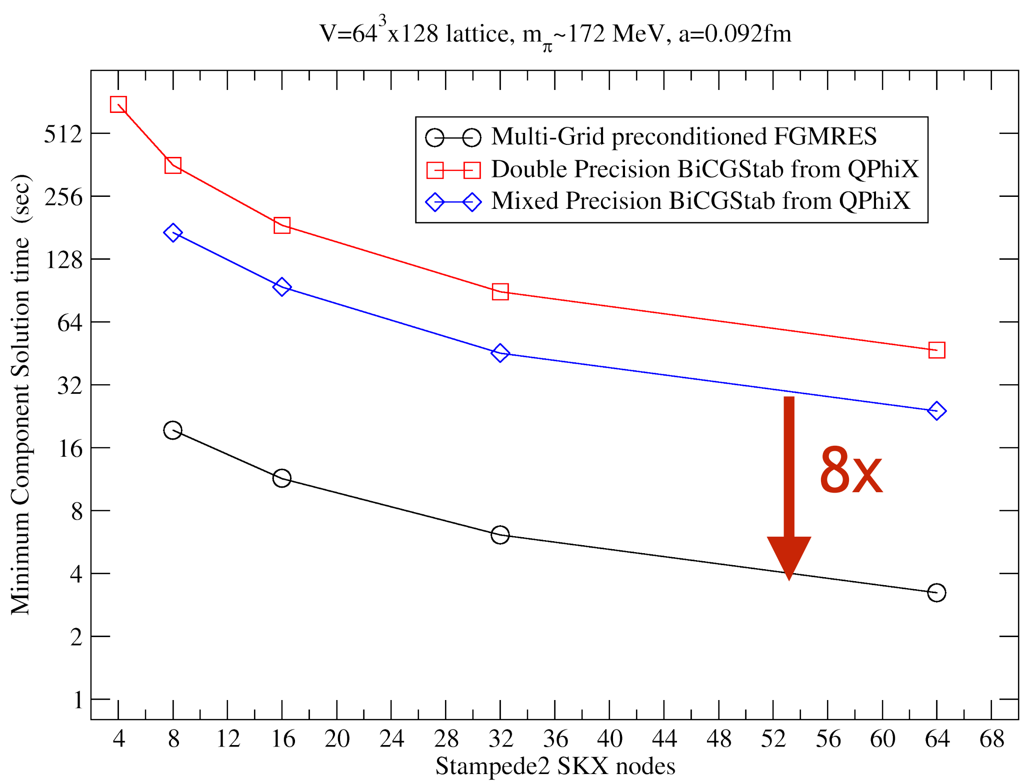
Accelerating propagators

Collaboration involving ASCR support and Industry partners

- O(1M) right-hand sides for Dirac equation per configuration
- Ill-conditioned solver at light quark masses
- Solution - Adaptive Multigrid (*QUDA & MG-PROTO*)

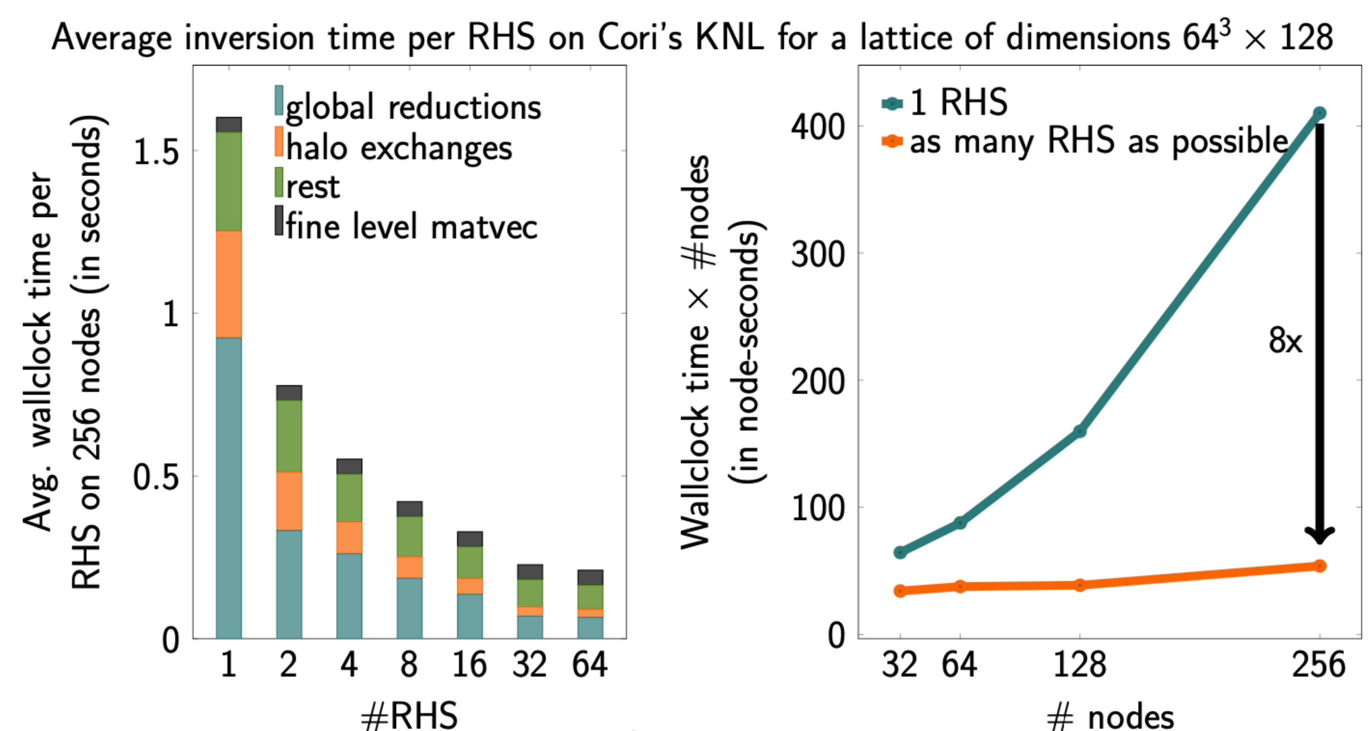


Stampede 2 (Skylake) - Strong scaling



8x speedup over conventional methods

Multiple right-hand sides



Another 8x speedup

64x speedup in total -> more science

Reducing contraction/correlator costs

Gauge generation
- Leadership level
- Strong scaling

Strong scaling limited
- Comms/compute less balanced in recent machines
- Latency in comms important
- Require comms reduced linear solvers
- 1-flavor solvers

Sympletic PDE integrators

Data-parallel code gen. with comms

Analysis
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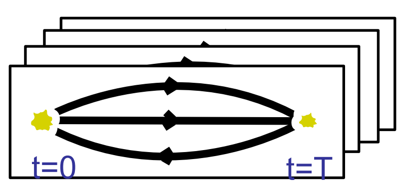
Contractions

Correlators
- O(1M)/cfg



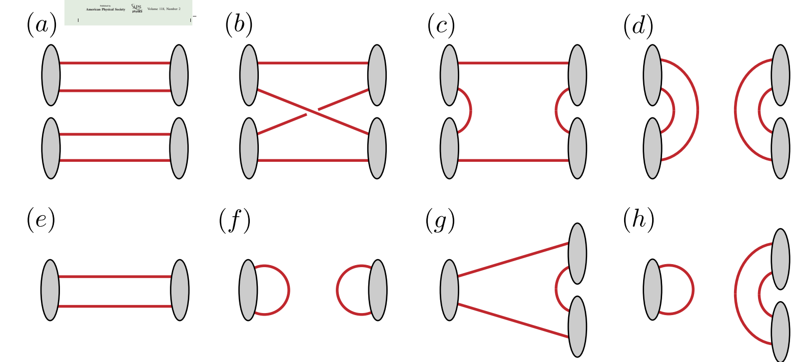
“Workflow” challenge
- Combinatorics -> improved graph theoretic methods
- Code generation for (sparse?) tensor contractions
- Job coordination -> Grid based

Redstar - workflow for many-body correlation functions

Collaboration involving ASCR support

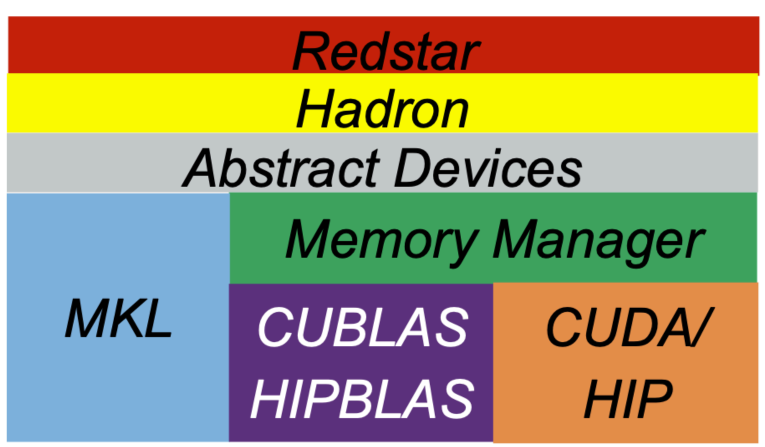
- Variational analysis of a matrix of correlation functions $C_{ij}(t) = \langle 0 | \mathcal{O}_i(t) \mathcal{O}_j(0) | 0 \rangle$
- Relies on an extensive basis of many-body quark field operators
- Combinatorics of quark connectivity grows significantly
  - E.g., “simple” $\pi - \pi$ system - products of “graphs”
  - Optimally evaluate O(1M) graphs - “tensor contraction”

HadSpec: Phys.Rev.D97 (2018); Phys.Rev.Lett.118 (2017)

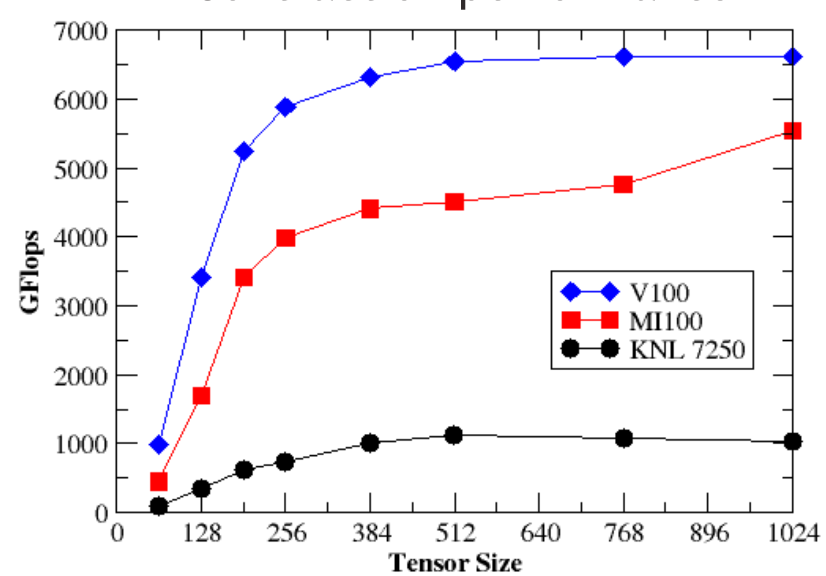


- ***Redstar*** (JLab) is a workflow engine using the “distillation” algorithm

Hierarchy



Contraction performance



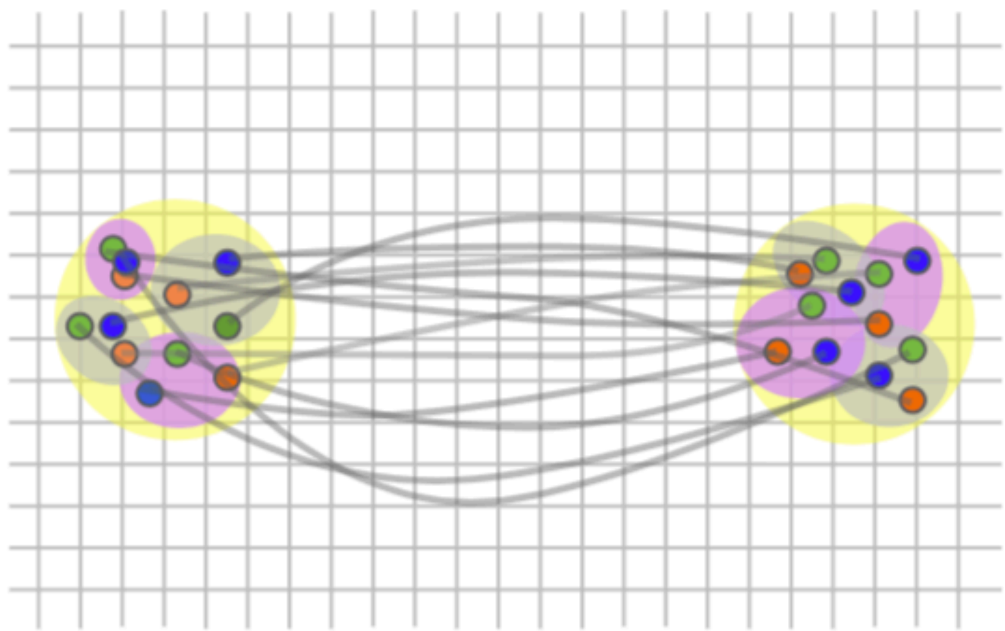
Hot off press:
4 - 6x speedup on GPU

Chroma & Redstar
(~)ready for Frontier

QCD for nuclei

- Quarks need to be tied together in all possible way

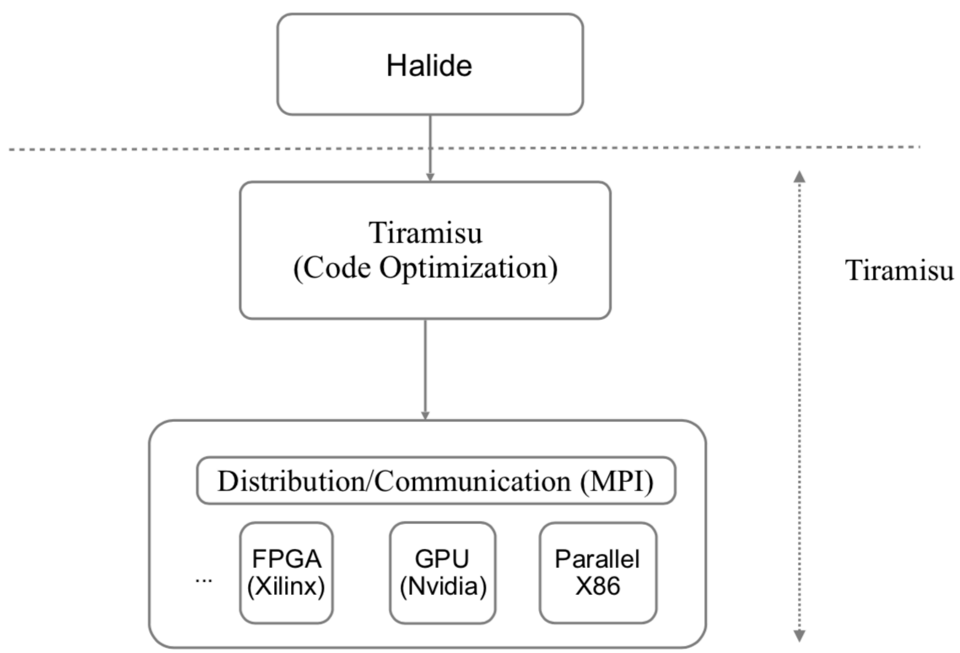
$N_{contractions} = N_u! N_d! N_s!$ $\quad (\sim 10^{1500}$ for $^{208}Pb)$

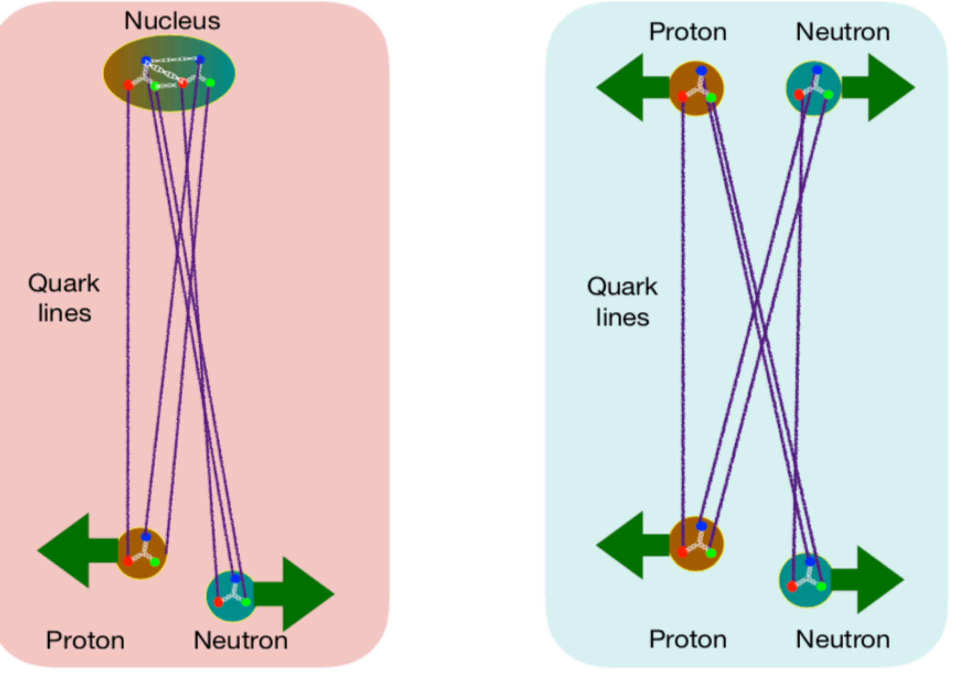


- Manage using algorithmic trickery - still significant graph contractions
- TACO @ MIT (cf TCE, Cyclops) http://tensor-compiler.org
  - general purpose tensor contraction compiler framework
  - target to QCD specific problems (sparsity patterns, …)
  - Allow efficient exploration of methodology

QCD for nuclei - Halide & Tiramisu

- Extend Tiramisu to accomodate LQCD & CUDA





- Proof of concept for conjugate-gradient inverter - **1.2x**
- Significant speedups for tensor-contraction construction - **90x**
- Open source release of the improved Tiramisu & Halide DSLs
- Automatic sparse tensors and optimizations

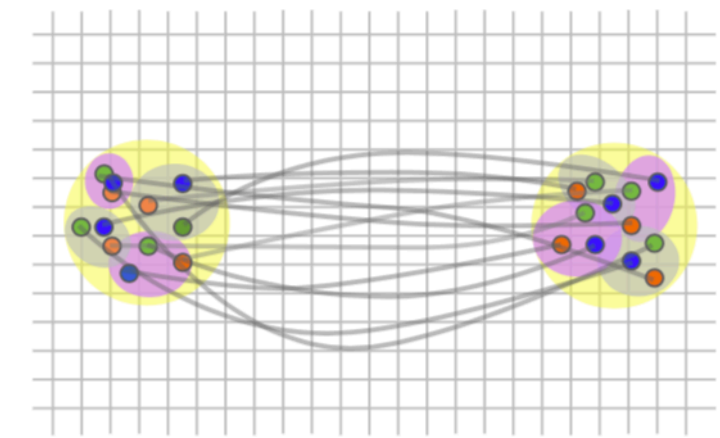
http://tensor-compiler.org

QCD for nuclei - going to physical quark masses

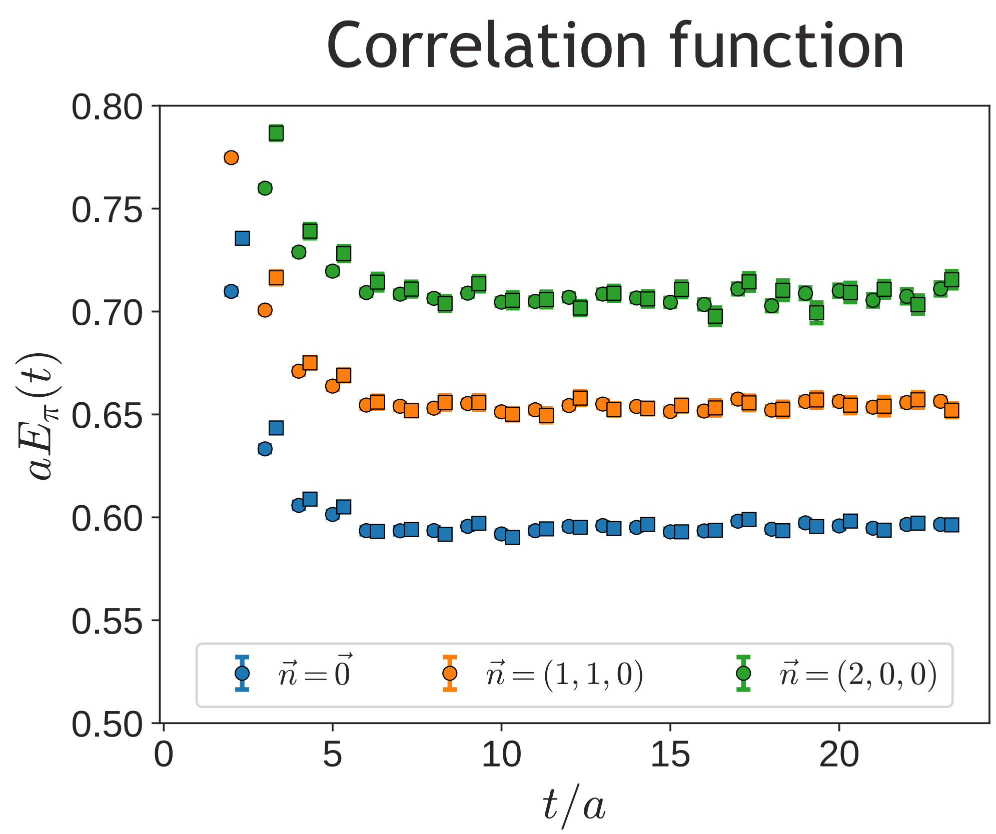
- Reduce the volume scaling cost by reducing the volume!

$N_{contractions} = N_u! N_d! N_s!$ $(\sim 10^{1500}$ for ^{208}Pb$)$

Restriction: Aggregation over sites



- Combine with optimized block constructions → substantially reduces cost

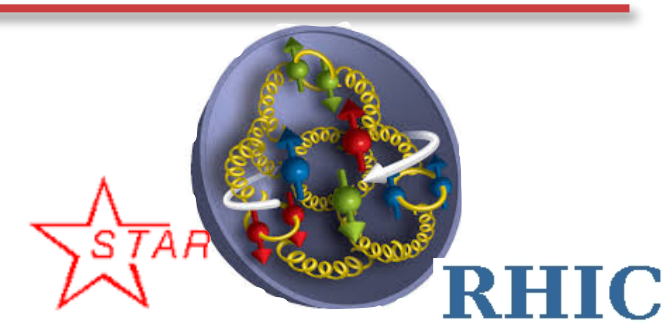


Sparse (▪) and full (●) effective energies for the pion at various different momenta

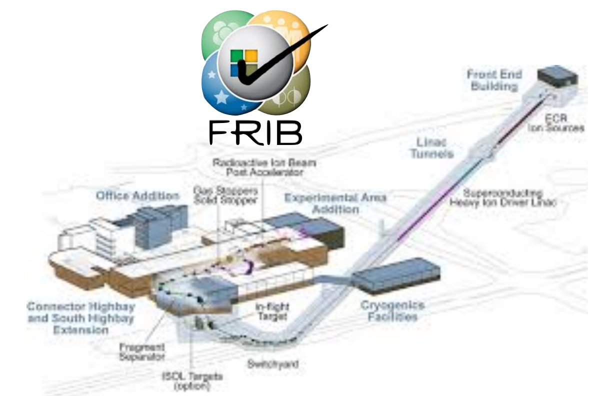
[arXiv:1908.0705]

LQCD focused on science and infrastructure

- LQCD provides interpretation to extreme matter @ RHIC



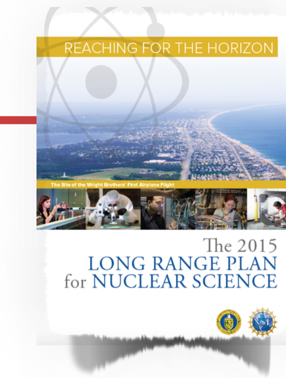
- Nuclear structure well aligned with FRIB and Fund. Sym.



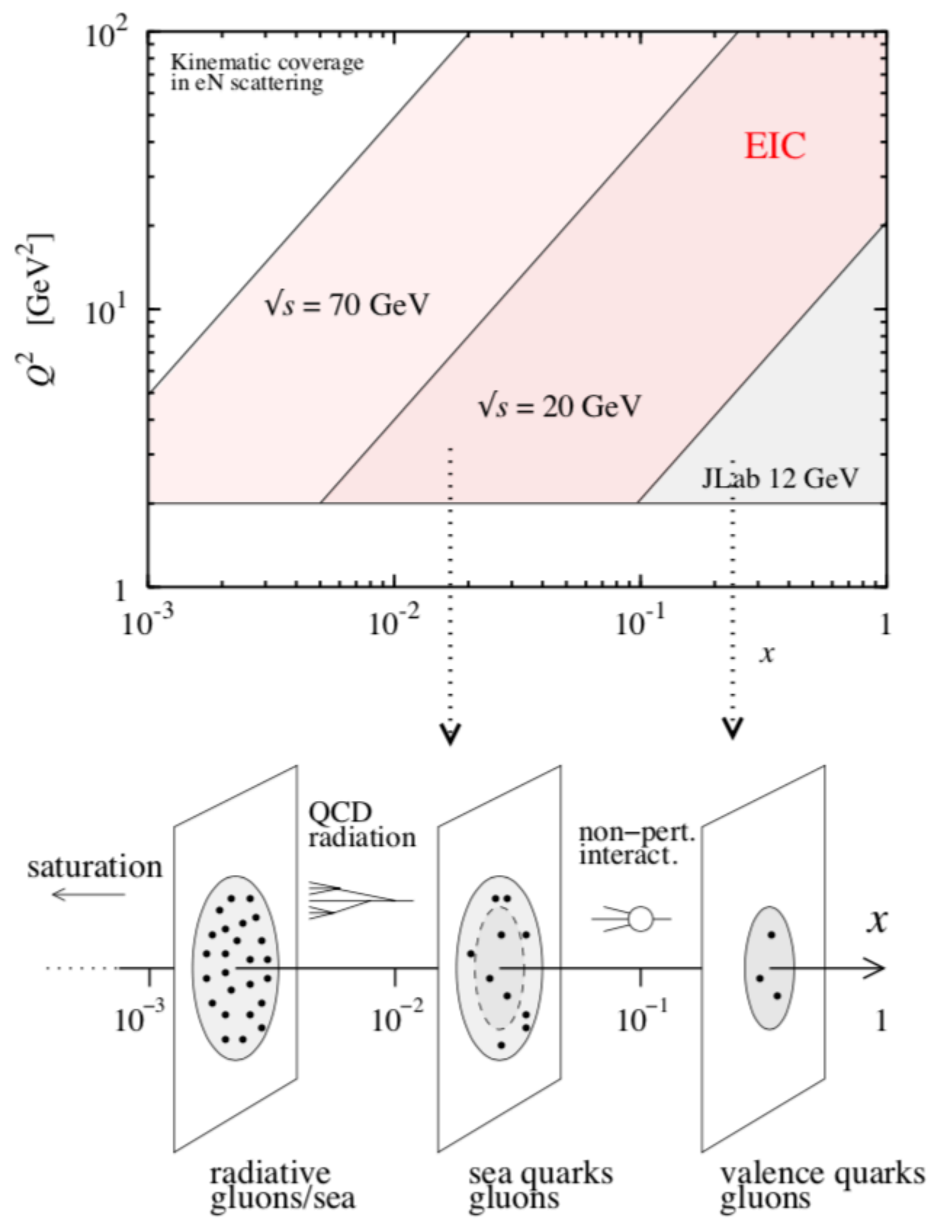
- Hadron spectroscopy and structure efforts align with JLab12
  - Guiding expt. searches at CLAS12 & GlueX

- But new opportunities…
  - Particular interest is role of glue in QCD

Electron Ion Collider in US



Particular interest is role of glue in QCD



Partonic structure of gluonic states complementary to such a program

Merging of spectroscopy and structure efforts

first baby-steps PRD98 014511 (2018)

Computer “measurements” beyond experimental reach

Computing at forefront

SciDAC-4 is a partnership

- Strong existing partnerships with ASCR & HEP supported community members

- 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

Work plan (as shown in mid-term review)

Year 1 | Year 2 | Year 3 | Year 4 | Year 5

Jefferson Lab

- Xeon Phi Multi Grid Solvers
- Multi-Grid Solvers: Perlmutter Readiness
- Multi-Grid Solvers Aurora & Frontier Readiness
- Multi Grid Solvers and Gauge Generation Summit Readiness
- Gauge Gen. Perlmutter Readiness
- Gauge Gen & Chroma readiness for Aurora & Frontier
- Force-Gradient Integrator. KNL Strong Scaling Optimization (+LANL)
- GWU Code Port to Aurora and Frontier
- Completion of work on QUARC (RENCI)
- QPerf: Memory optimization tool development and application to LQCD (W&M)

MIT

- Halide: Preliminary Infrastructure and Initial Investigation
- Halide:USQCD Code Base Integration
- Halide and Multi-Node Optimizations for LQCD
- Halide code generator and new architectures
- Interface DeepHyper with USQCD software (was OpenTuner)
- Apply Autotuning for Source Construction
- Database Technology for contraction storage(+UW/PNNL)
- Contractions and TACO: Initial infrastructure
- Action Matching Using Machine Learning (New)
- Generalized SVD Complexity Reductions (+UW/PNNL)
- Determinental Nuclear Contractions (+UW/PNNL)
- QLUA Improvements and HMC (New)
- Apply TACO to graph theoretic contraction approaches
- Optimize Contraction codes for KNL and GPU (+UW/PNNL)
- Data reduction, sparsification and approximation strategies (+ UW/PNNL)
- Hierarchical Multi-Level QLua

BNL

- PanDA Workflow at OLCF Titan & Summit
- PanDA Workflow at ALCF Systems & NERSC
- Single Node HiSQ Code for Summit
- Optimize Single Node HiSQ for Perlmutter
- Optimize Single Node HiSQ for Aurora
- Multi-GPU HiSQ code for Summit
- Multi-Node HiSQ Code for Perlmutter
- Multi-Node HiSQ Code for Xeon Phi, Aurora readiness
- Single node Anisotropic HiSQ (aHisQ) on Cori and Summit
- Multi-Node aHiSQ code on Perlmutter
- Multi-Node aHiSQ code on Summit and Aurora

Milestones (midterm review)

Gauge generation and Solvers (under co-PI - Balint Joo)

JLab, UNC, LANL, W&M, GWU

Table 4: Revised Milestones for Gauge Generation and Solvers; Participants are BJ=Bálint Joó, BJR = Bálint Joó replacement, FW=Frank Winter, KC=Kate Clark, BY=Boram Yoon, AA=Andrei Alexandru, P=Postdoc (JLab), FW=Frank WInter, ER=Eloy Romero (W&M Postdoc), WS=Wei Sun (JLab Postdoc), ER= Eloy Romero (W&M Postdoc), RB = Ruairi Brett (GWU Postdoc), G2=Graduate Student (W&M). Status codes: C=Completed, P=Progressing, NS=Not Started, D=Descoped, R=Rescoped. We show also the original milestones from 3 to which the new milestones correspond in the second column.

ID	Original ID	Year	Milestone	Participants	Status
R1	2	3	Multi-RHS Multi-Grid Solver Implementation in QUDA	KC	P
R2	8	3	Xeon Multi-Grid Solver Multi-RHS	ER/BJR, ER	P
R3	9	3	Integrate QUDA Multi-RHS solvers into Gauge Generation on Summit	BJ/BJR, KC, WS	NS
R4	14	3-4	Multi-Grid Solvers, Frontier and Aurora Readiness (under ECP)	BJ, BJR, KC	P
R5	12	3-4 .	Port QDP-JIT/LLVM Frontier and Aurora (under ECP)	FW	P
R6	new	4	Add exponentiated Clover formalism into QUDA	KC, BJR	NS
R7	new	4	Add exponentiated Clover formalism into Chroma	BJ/BJR, WS, ER	NS
R8	new	4	Integrate R6 and R7	KC, BJ, BJR	NS
R9	24	4	Finish fine grained profiling component of QPerf	XL, G2	NS
R10	16,22	4-5	Porting of GWU code to Aurora and Frontier	AA, RB, BJ	NS / R
R11	new	5	Demonstrate Kokkos optimization of loop fusion for select Chroma measurements	BJR, WS, ER	NS
R12	26	5	Use QPerf to analyze memory patterns of LQCD Codes on Aurora, Perlmutter	XL, BJR, G2	NS

Milestones (midterm review)

Contractions (under co-PI - Will Detmold)

MIT & PNNL

Table 6: Revised Milestones for Contractions; Participants are SA=Saman Amarasinghe, WD=William Detmold, AP=Andrew Pochinsky, RB=Riyadh Baghdadi, KR=Kenneth Roche, JS=Jan Strube, P=postdoc, G=graduate student. Status codes: C=Completed,P=Progressing, NS=Not Started, D=Descoped, R=Rescoped, N= New

ID	Year	Milestone	Participants	Status
C1	1	Preliminary interfacing of Halide/Tiramisu with LQCD Codes	–	C
C2	1	Target Halide /Tiramisuto write concrete LQCD Kernels	–	C
C3	1	Begin Interfacing OpenTuner to USQCD Software	–	R,C
C4	1	Understand How Contraction Tasks Map onto TACO	–	C
C5	1	Optimize Specific Nuclear Physics Contractions on KNL and GPU	–	C
C6	2	Investigate Halide Code Generation for KNL	–	D
C7	2-3	Improve Halide/Tiramisu Integration with USQCD Code	SA, RB, AP, G	P
C8	2	Test Autotuning Framework for Multigrid Parameter optimization	WD, G	P
C9	2	Improve OpenTuner Interfaces	WD, G	R
C10	1-2	Action matching using machine learning	–	N,C
C11	1-2	QLUA improvements and HMC	–	N,C
C12	2-4	Investigate Data Reduction, sparsification and approximation approaches	–	C
C13	3	Apply Autotuning to Gauge Generation	AP, WD	NS
C14	3	Investigate Generalized SVD Complexity Reduction	WD, KR, JS	NS
C15	3-4	Apply Halide/Tiramisu to multi-node optimizations	SA, RB G	P
C16	3-5	Apply autotuning to Source Construction	WD, AP, G	P
C17	3-5	Investigate database technologies for storing contraction Data	KR, JS	P
C18	3-5	Apply TACO to graph theoretic approaches	SA, G	NS
C19	3-5	Hierarchical multilevel QLUA	AP	N,NS
C20	4-5	Determinantal nuclear contractions	WD,AP,KR,JS	N,NS

Milestones (midterm review)

Extreme matter (under co-PI -
BNL & Michigan State U.

Table 5: Year 4-5 Milestones for BNL part of the project. C=Complete, P=In Progress, R=Rescoped, NS=Not Started, PD=Postdoc, GS=Graduate student, SM=Swagato Mukherjee, AB=Alexei Bazavov.

ID	Year	Milstone	Participants	Status
		Original		
T1	4-5	Single-node HISQ for NERSC-9	SM, GS	C
T2	4-5	Multi-node HISQ for NERSC-9	SM, PD	C
T3	4-5	Multi-Node aHISQ code on NERSC-9	AB, PD	P/R
T4	4-5	Multi-Site PanDA Workflow	PD	C
		New		
T5	4-5	Aurora readiness for HISQ code	SM, PD, GS	P
T6	4-5	Aurora readiness aHISQ code	AB, PD	P
T7	4-5	Frontier readiness for HISQ code	SM, PD	NS