

# Lattice Quantum Chromodynamics Project

SciDAC-4

**Robert Edwards  
Jefferson Lab**

# LQCD ASCR/NP SciDAC-4

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## 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

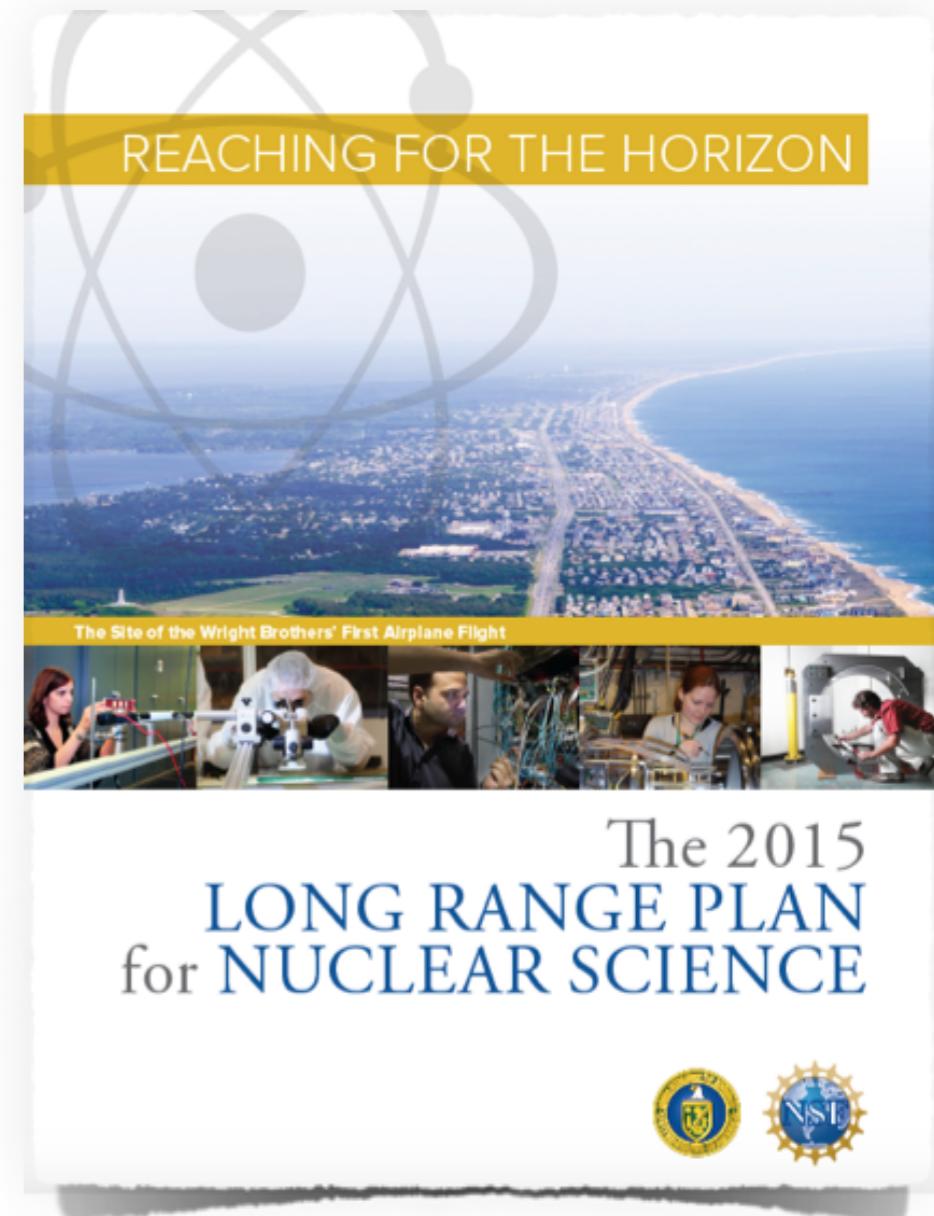
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## Long term collaborations with ASCR supported community and Industry

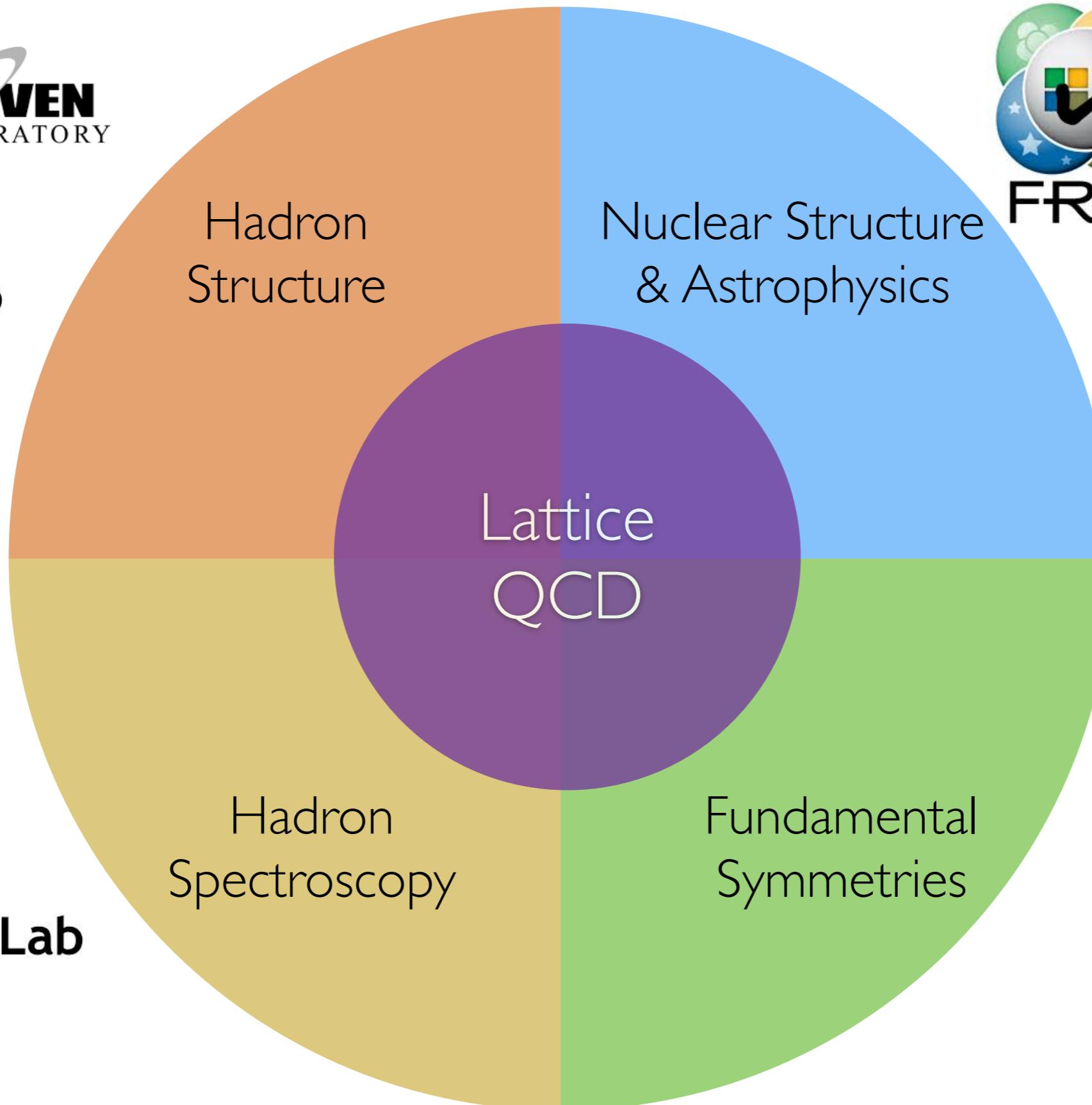
- Gauge generation (co-PI: Balint Joo)
  - **Balint Joo** - Sparse linear system solvers on emerging LCF-s (Cori, Summit, NERSC-9)
  - **Boram Yoon** - Symplectic PDE Integrators
  - **Kate Clark (NVIDIA)** - comms reduced solvers, Integrators
  - Kostas Orginos - 1 flavor methods
  - **Xu Liu** - Memory optimizations (QPerf and HPC Toolkit)
  - **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
  - **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

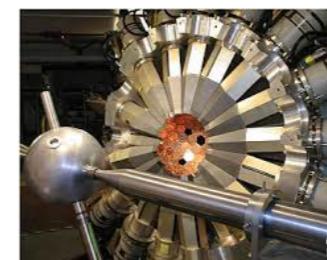
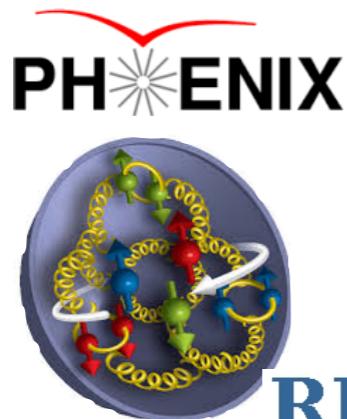
- Goals for field set out in 2015 NSAC Long Range Plan
  - JLab 12GeV: hadron spectroscopy and quark structure
  - FRIB: nuclear interactions, nuclear astro, fundamental symmetries
  - $\beta\beta$  decay: potential for LQCD input
  - EIC: gluonic structure of nucleons and nuclei
- Central to USQCD planning
- Experiment recognizes importance of computational NP initiative



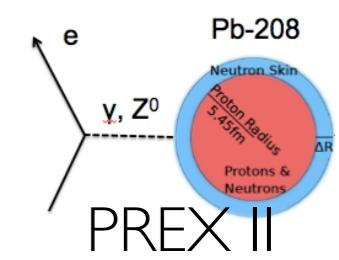
# Hadrons and Nuclei



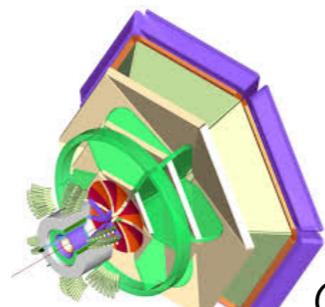
# LQCD/NP Science & connection to Expt.



Argonne  
NATIONAL LABORATORY



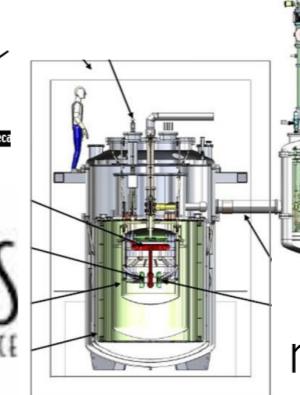
Jefferson Lab



CLAS12



npd $\gamma$



nEDM



PAUL SCHERRER INSTITUT

PSI

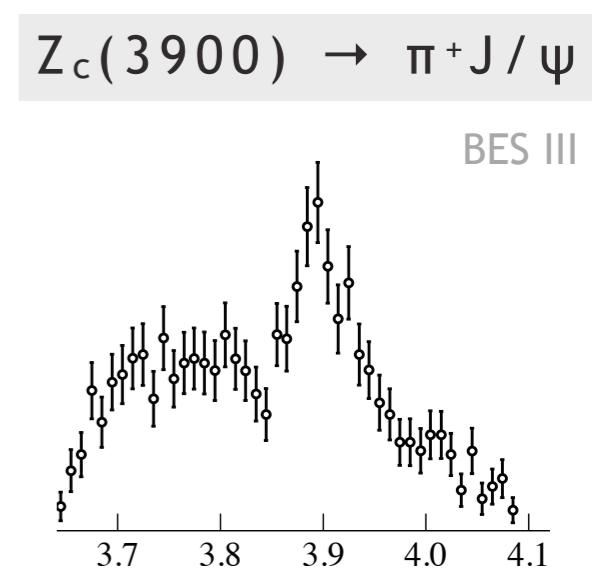
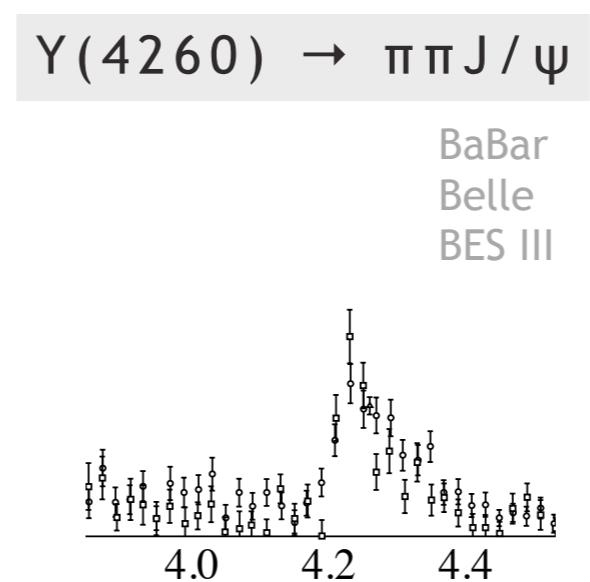
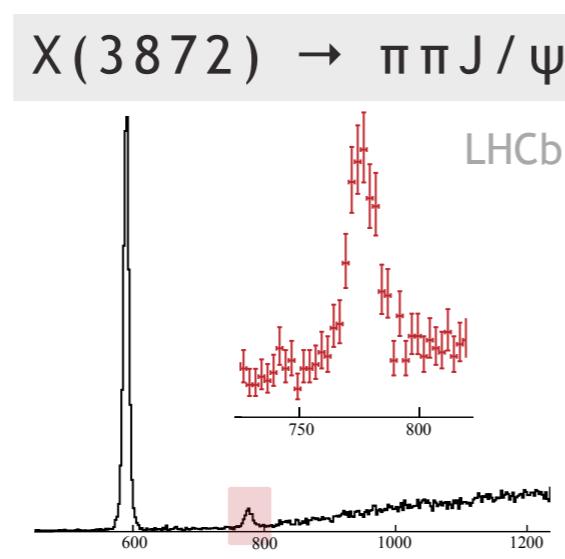


MuSUN

# 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 ?



# 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

**$f_0(500)$  or  $\sigma$**  [g]  
was  $f_0(600)$

$I^G(J^{PC}) = 0^+(0^{++})$

**$f_0(980)$**  [j]

$I^G(J^{PC}) = 0^+(0^{++})$

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

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

**$K_0^*(800)$**   
or  $\kappa$

$I(J^P) = \frac{1}{2}(0^+)$

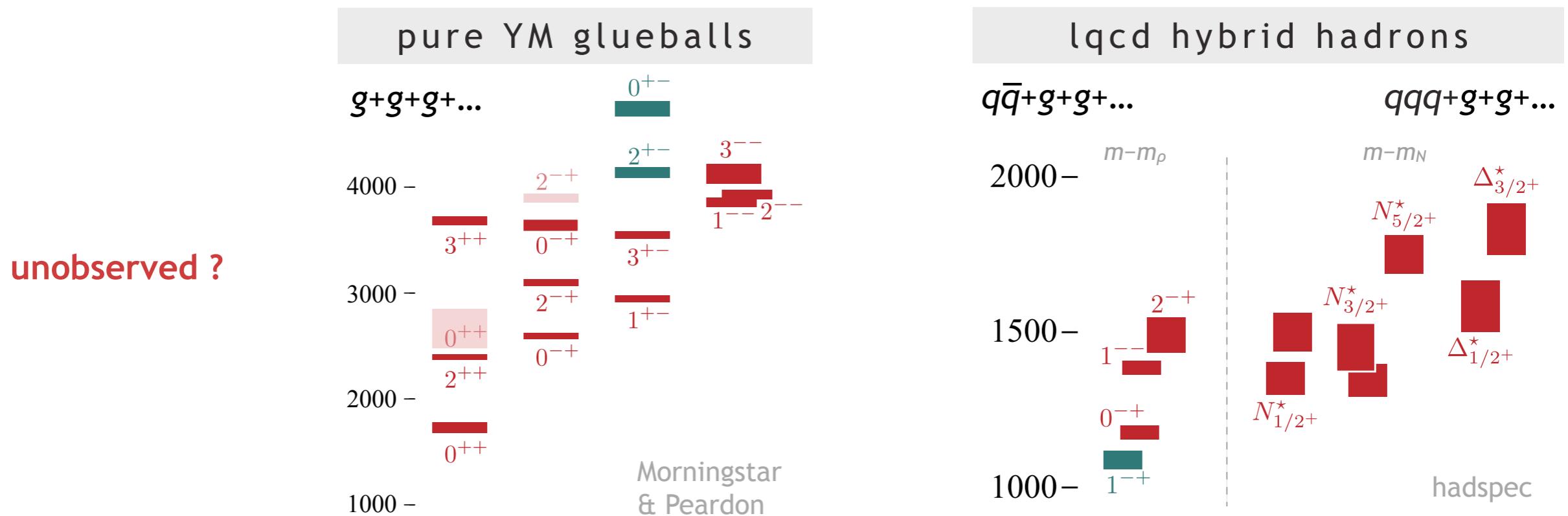
**$a_0(980)$**  [j]

$I^G(J^{PC}) = 1^-(0^{++})$

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

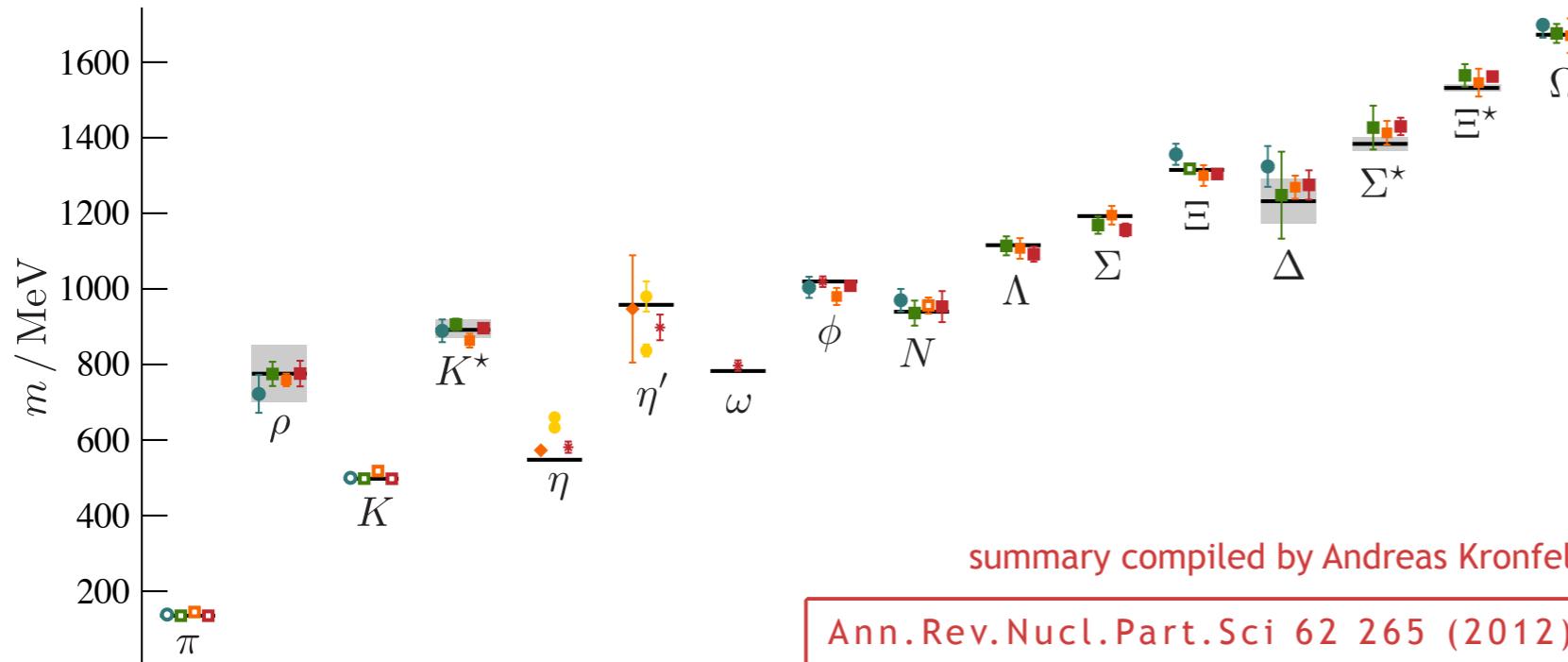
# QCD, hadrons and the standard model

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# Precise spectroscopy of stable hadrons

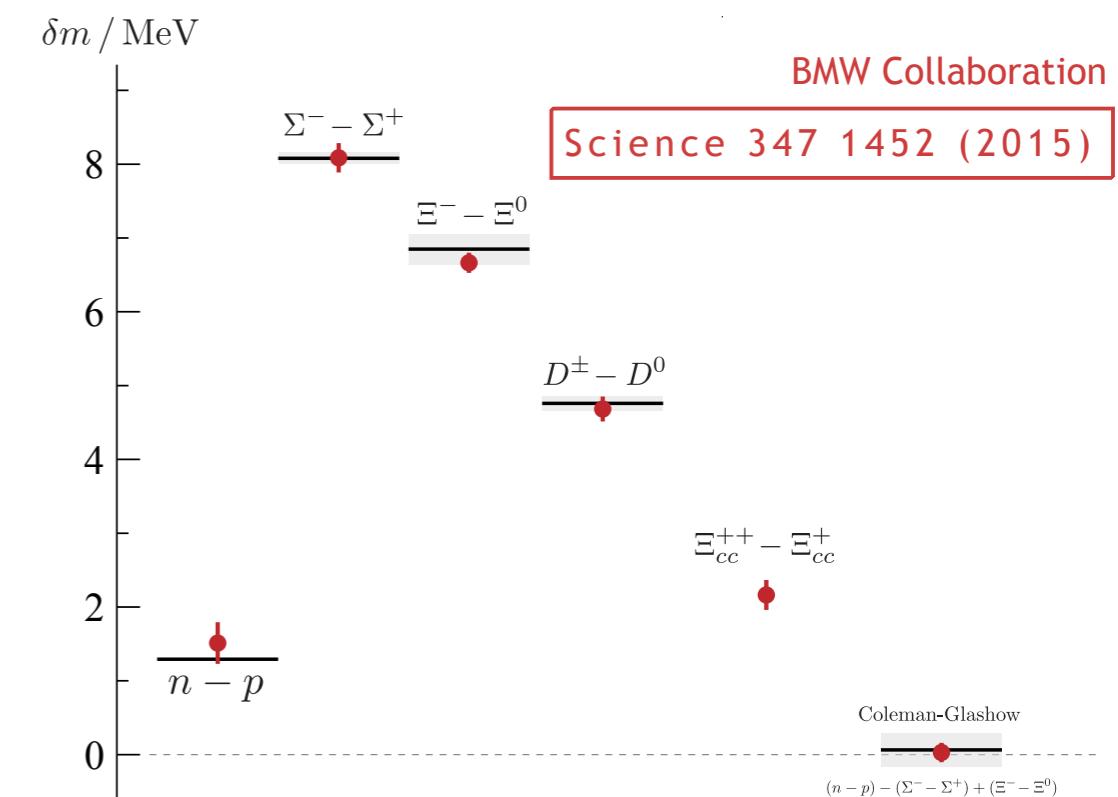
lattice qcd light hadron spectrum



summary compiled by Andreas Kronfeld

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

## QCD+QED mass shifts



Coleman-Glashow

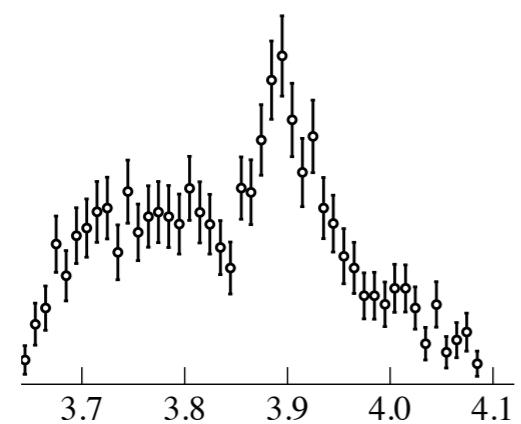
$$(n - p) - (\Sigma^- - \Sigma^+) + (\Xi^- - \Xi^0)$$

# Excited spectroscopy

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

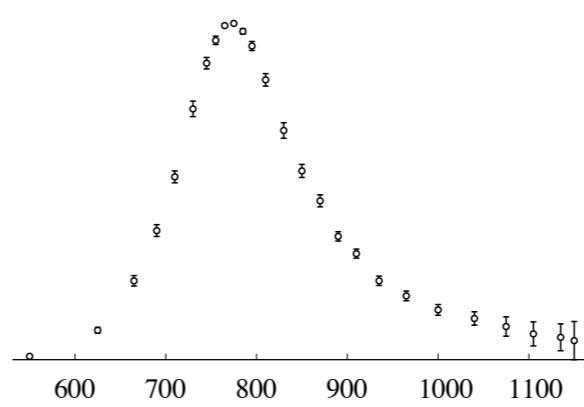
and they are **resonances** observed through their decays

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



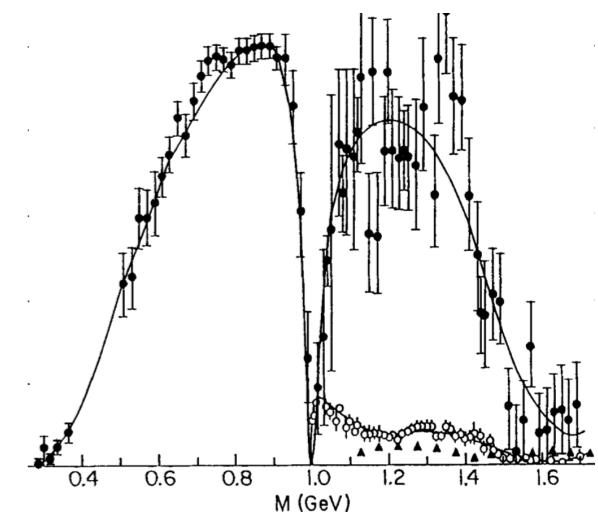
*exotic*

$\rho \rightarrow \pi\pi$



*familiar*

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



*non-trivial*

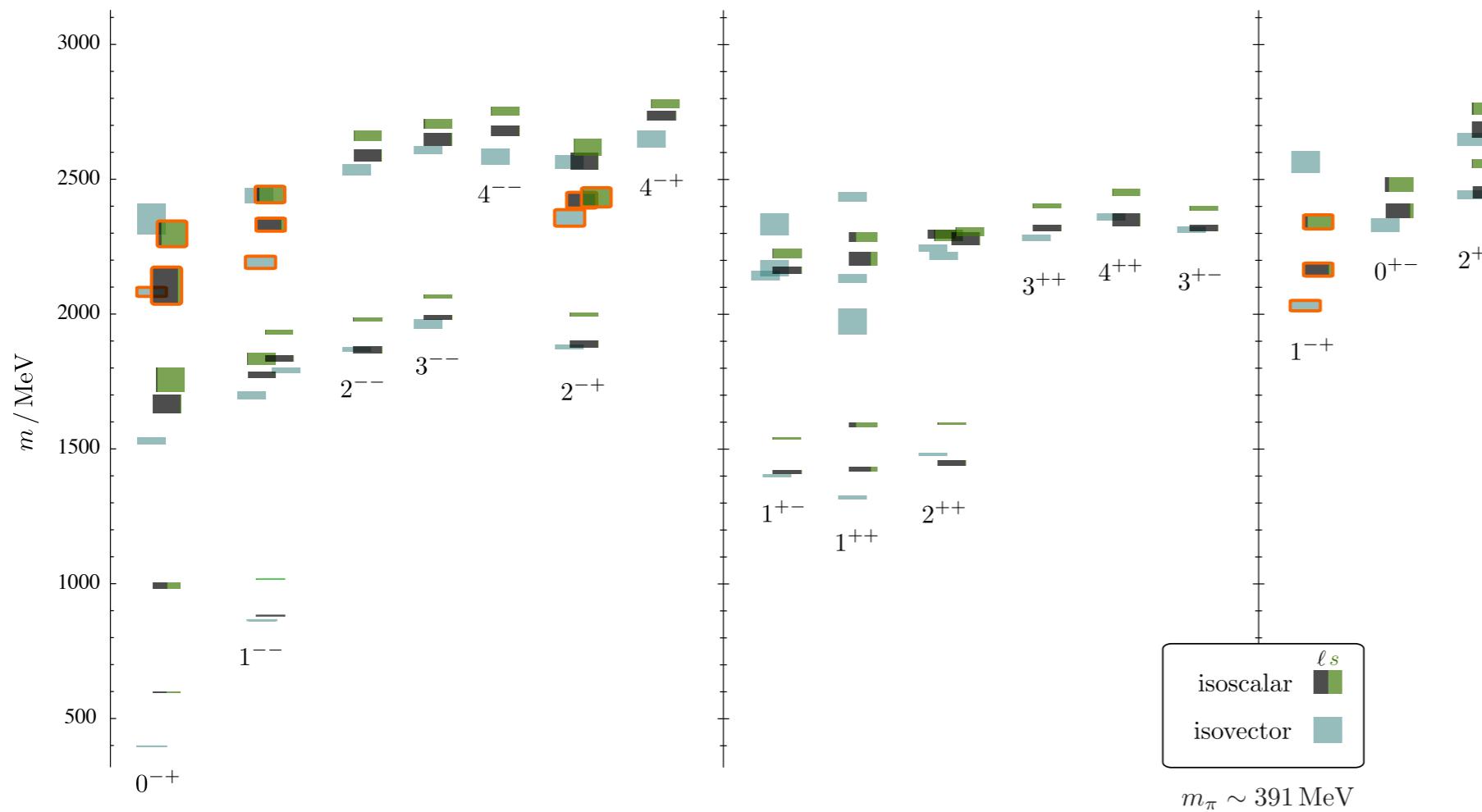
same non-perturbative dynamics **binds** and causes the **decay** – can't be separated within QCD ...

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

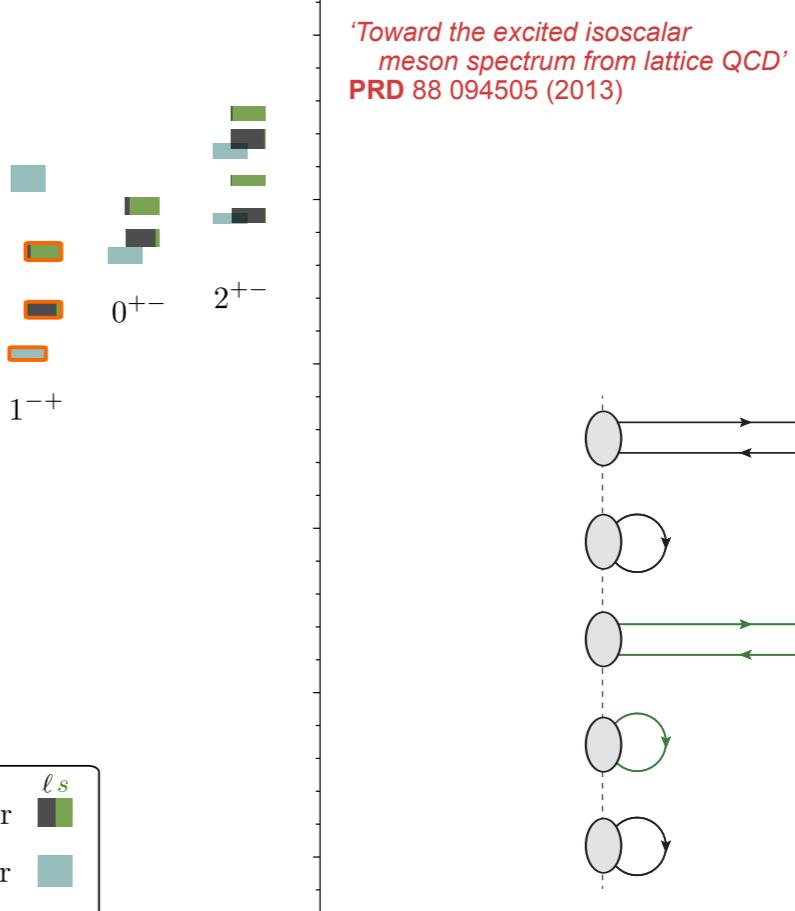
# Lattice QCD & the excited hadron spectrum

LQCD SciDAC project has pioneered novel techniques in lattice QCD

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



clear indication of a spectrum of hybrid mesons



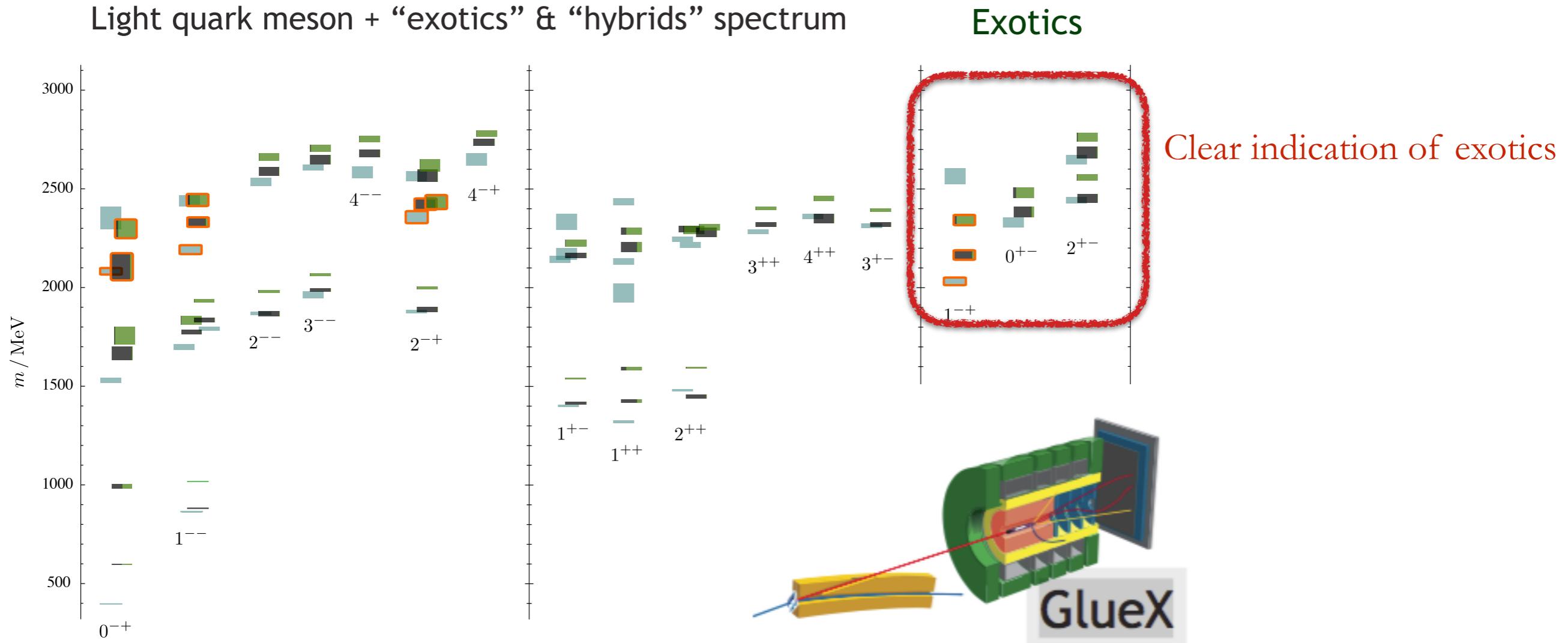
high precision calculation of  
disconnected diagrams

early adopters of GPUs



# Hadron Spectroscopy - role of the glue

Focus of GlueX & CLAS12 @ JLab & COMPASS, LHCb @ CERN, BES @ Beijing



→ Need to know decay modes and rates to compare to expt.

# Where are the “Missing” Baryon Resonances?

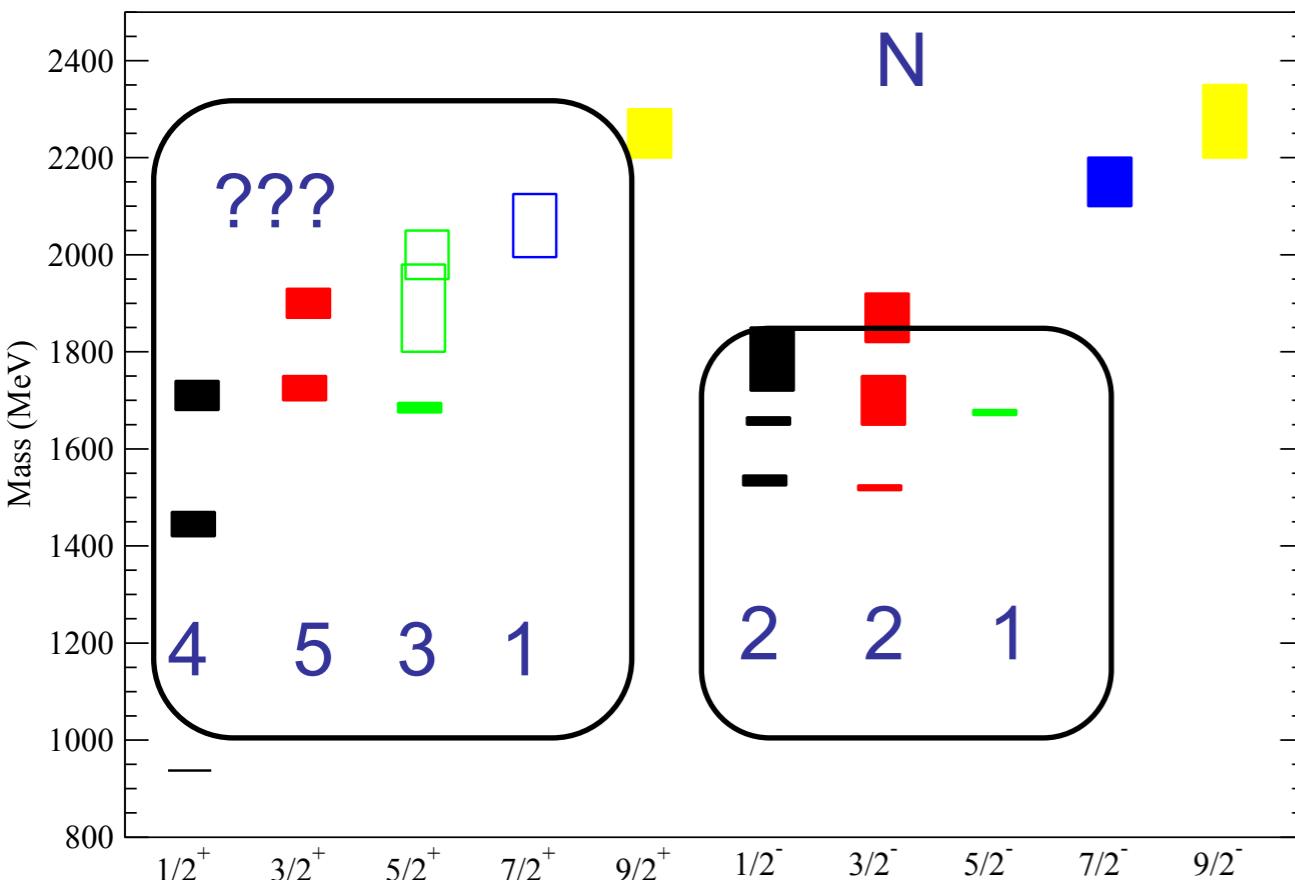
Only few found in expt. - thought that they were missing?

Theory/symmetries wrong?

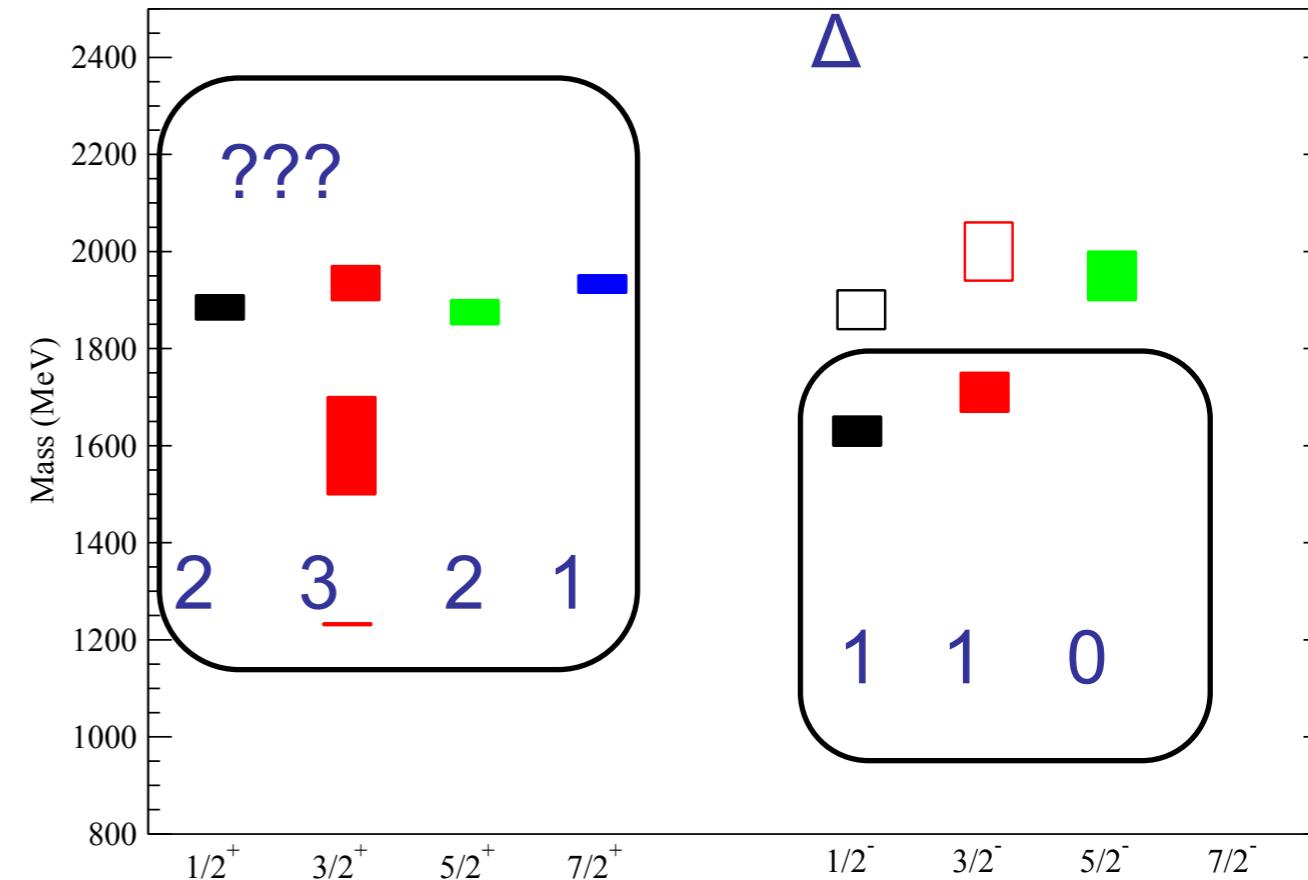
Nucleon & Delta spectrum  
PDG uncertainty on  
B-W mass

Expt. vs. predictions

Nucleon (Exp): 4\*, 3\*, some 2\*

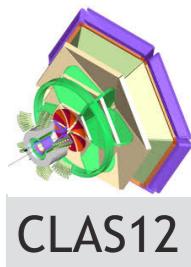


Delta (Exp): 4\*, 3\*, some 2\*

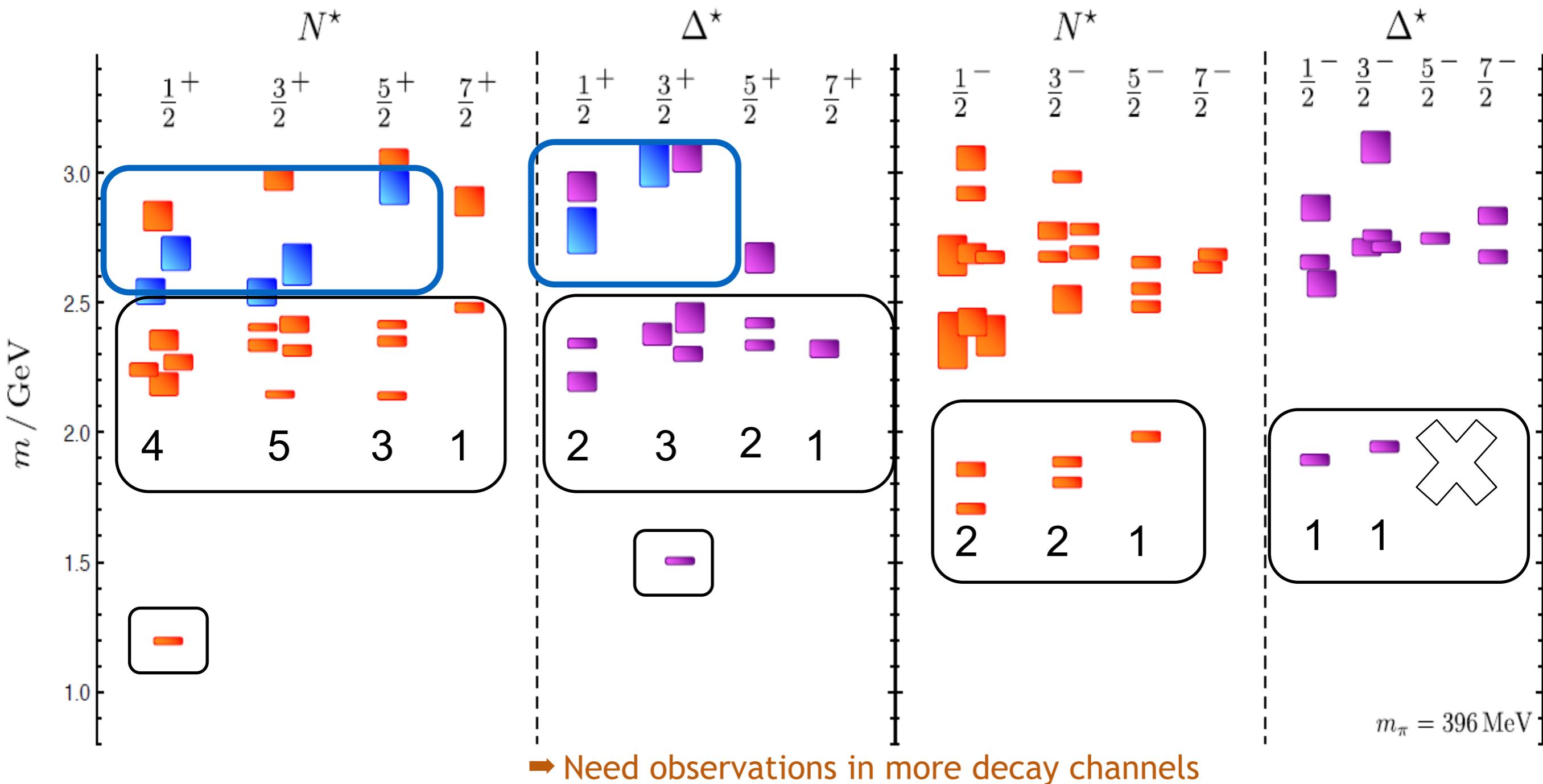


# LQCD suggest no “missing” baryon states

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

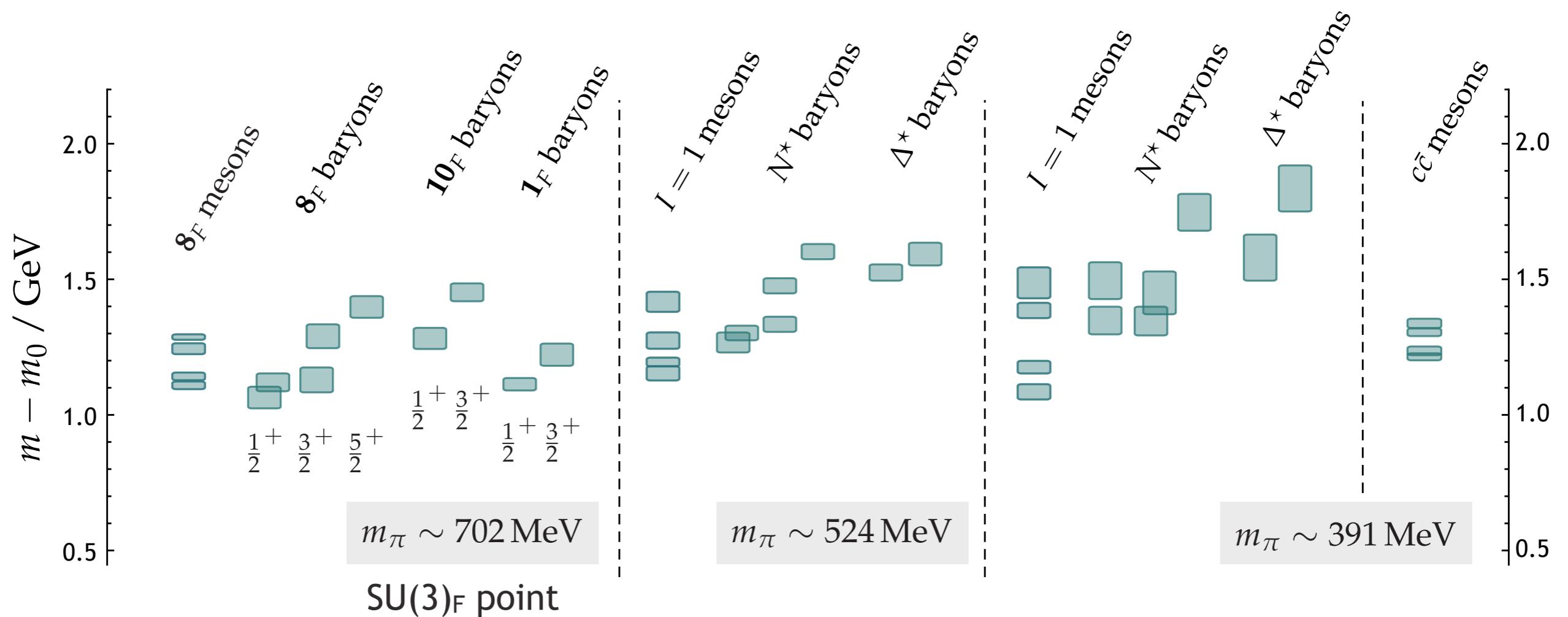


Additional gluonic excitations within baryons  
Spurred new expt. search in CLAS12@JLab



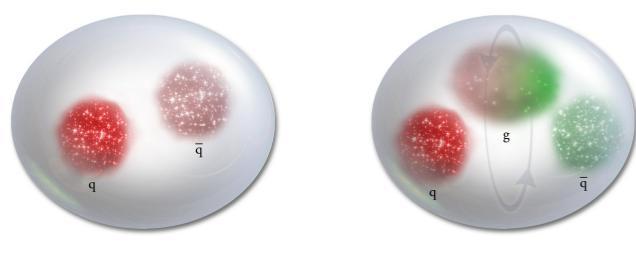
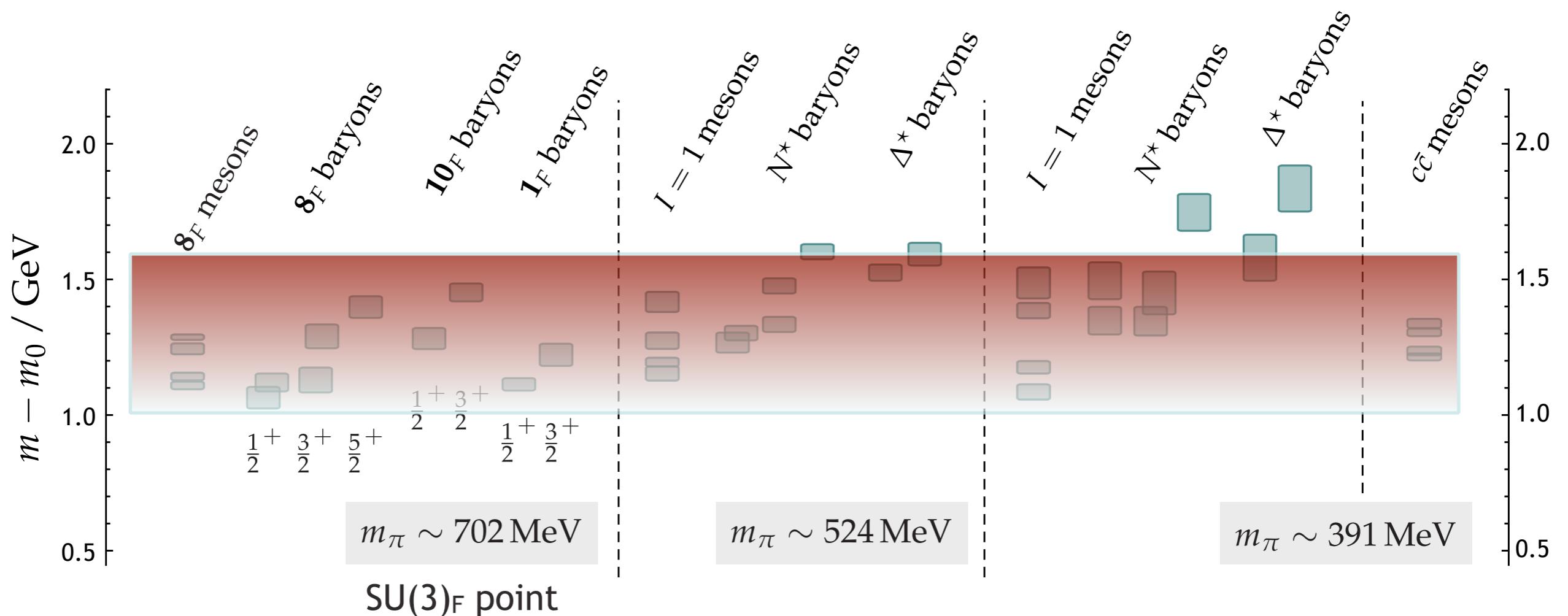
# Hadron Spectroscopy - role of the glue

- Subtract the ‘quark mass’ contribution



# Hadron Spectroscopy - role of the glue

- Subtract the ‘quark mass’ contribution

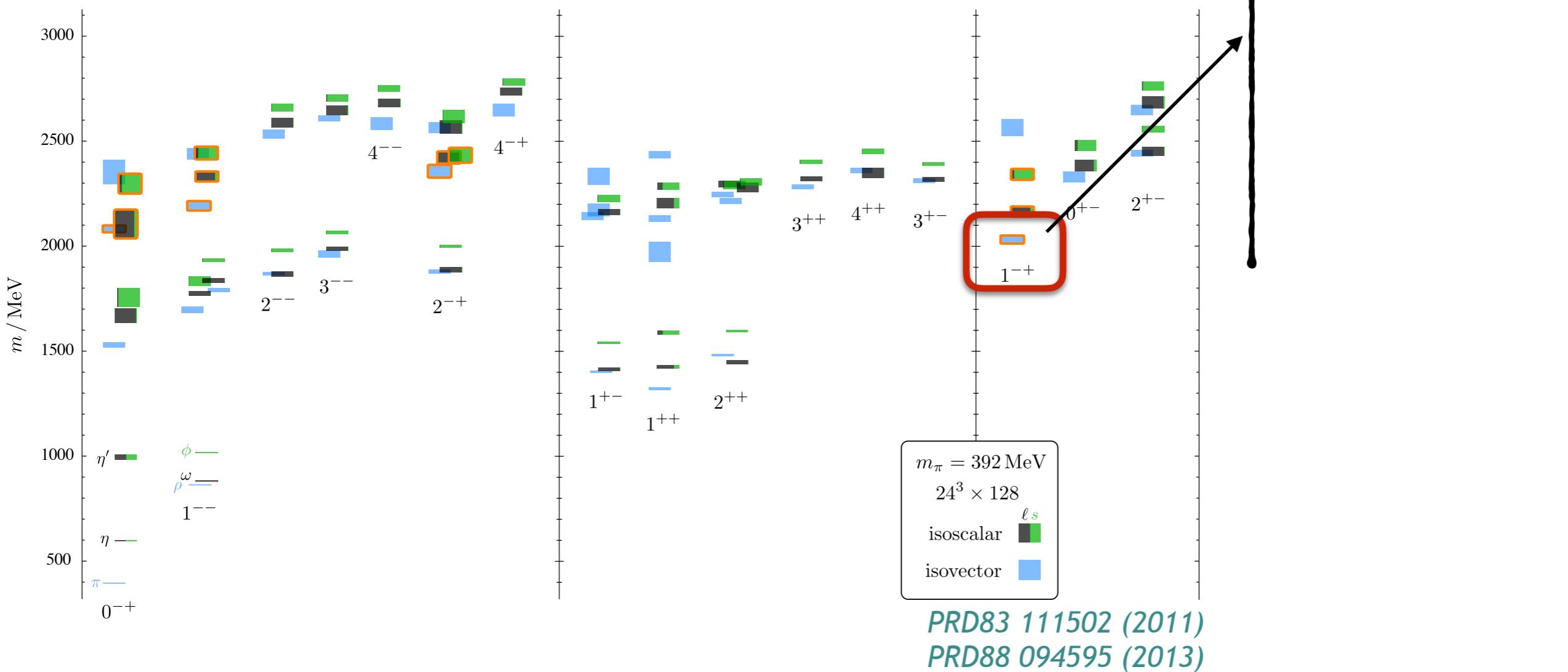


Common energy scale of gluonic excitation  $\sim 1.3 \text{ GeV}$

# Exotic hybrid mesons in QCD?

To predict and understand hybrid mesons from QCD

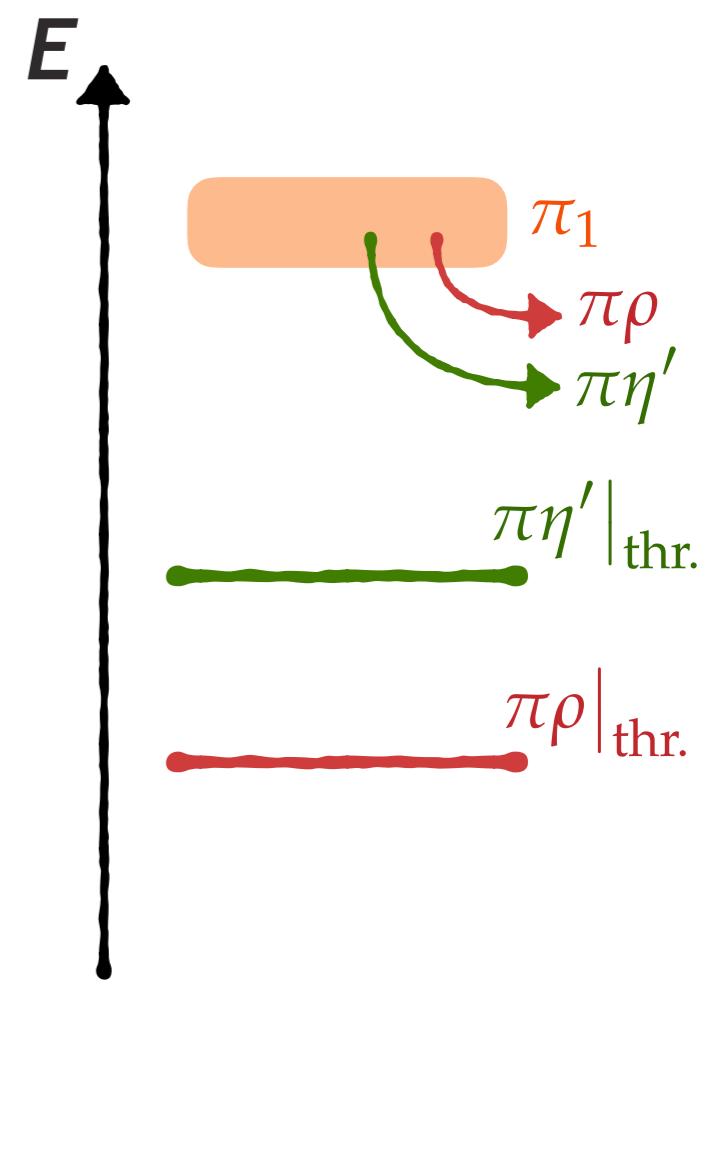
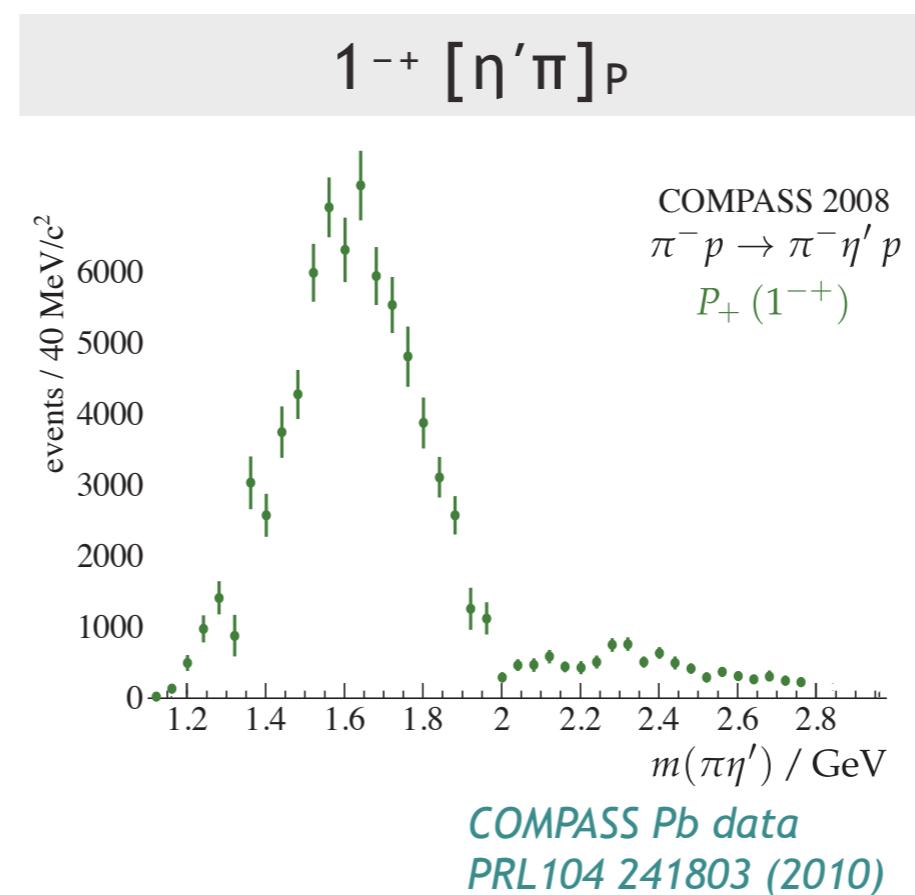
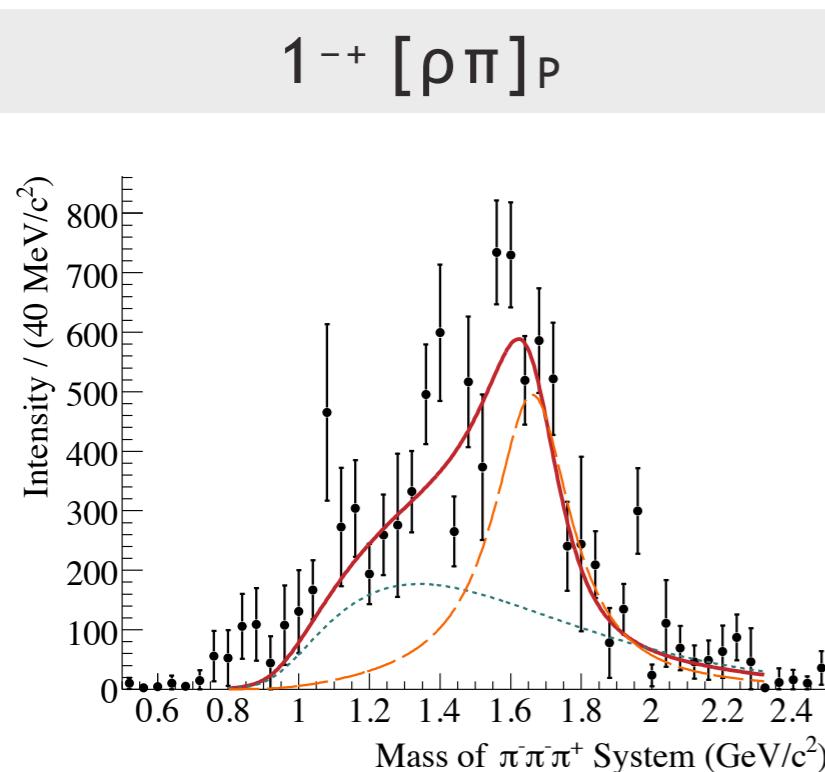
→ must predict decay modes



# Exotic hybrid mesons in QCD?

Excited states are resonances in scattering of lighter hadrons

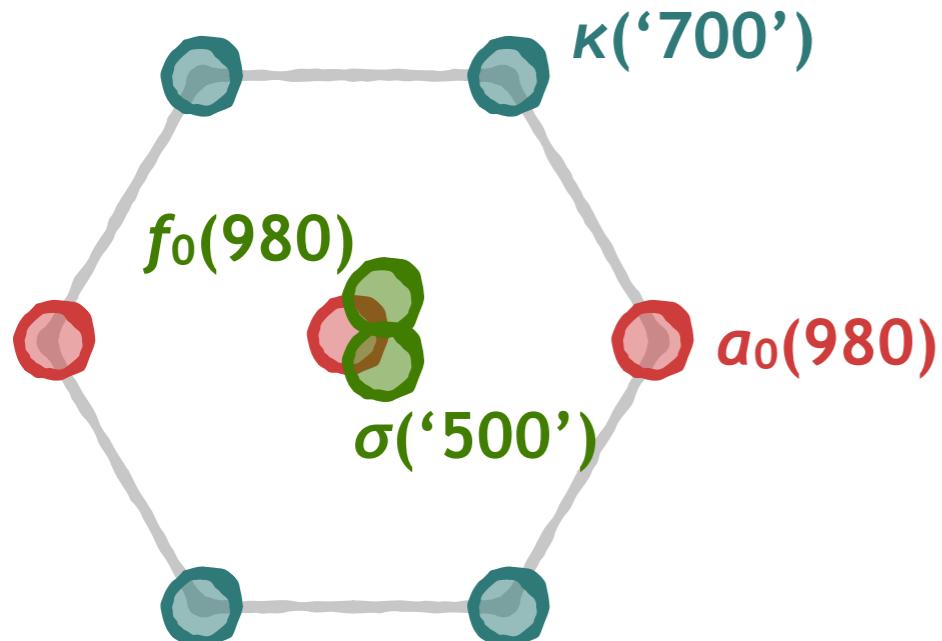
We should see this in LQCD



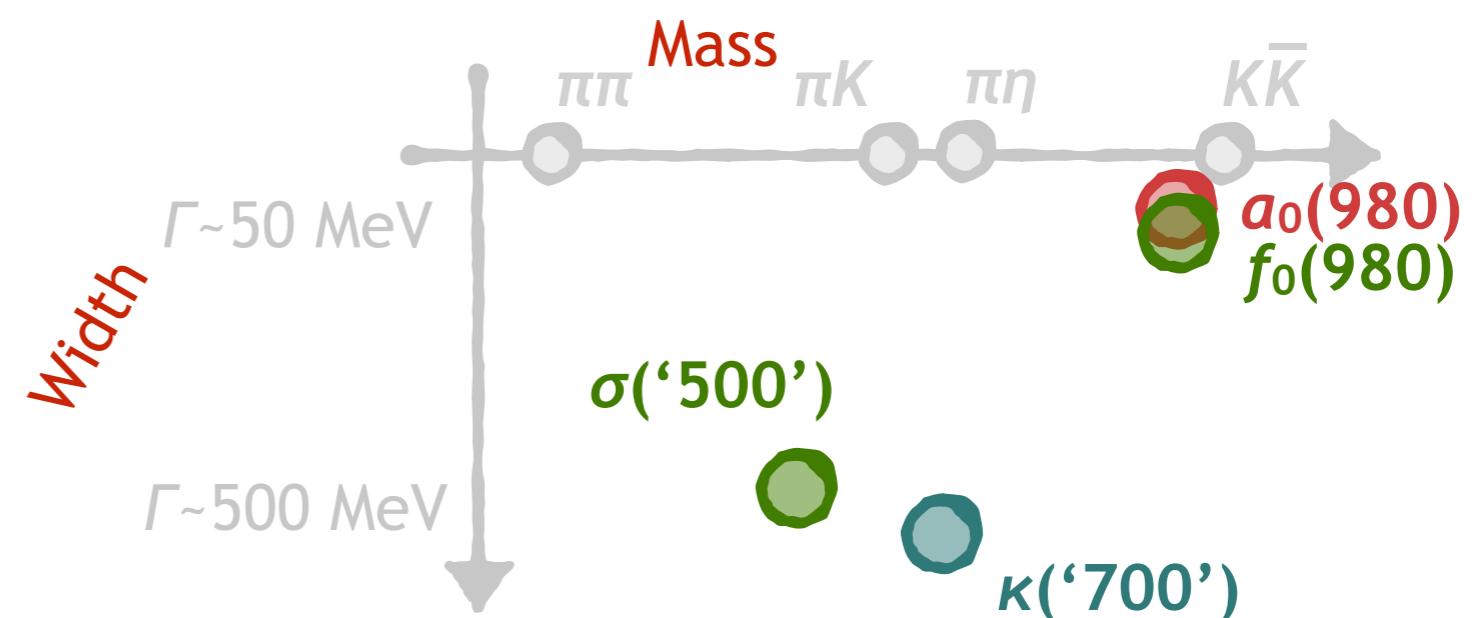
Hard - start with lower energies

# Mysterious light scalar mesons

Conventional wisdom: an ‘inverted’ mass nonet



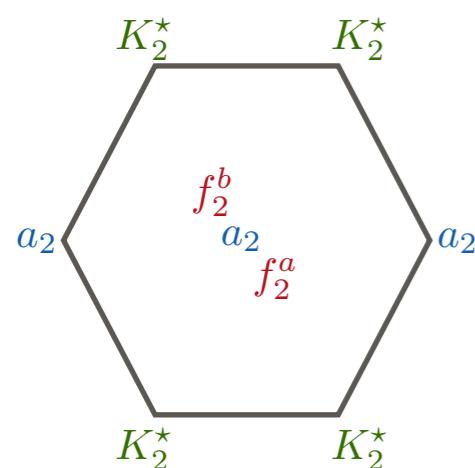
Similar? Vastly different masses & widths



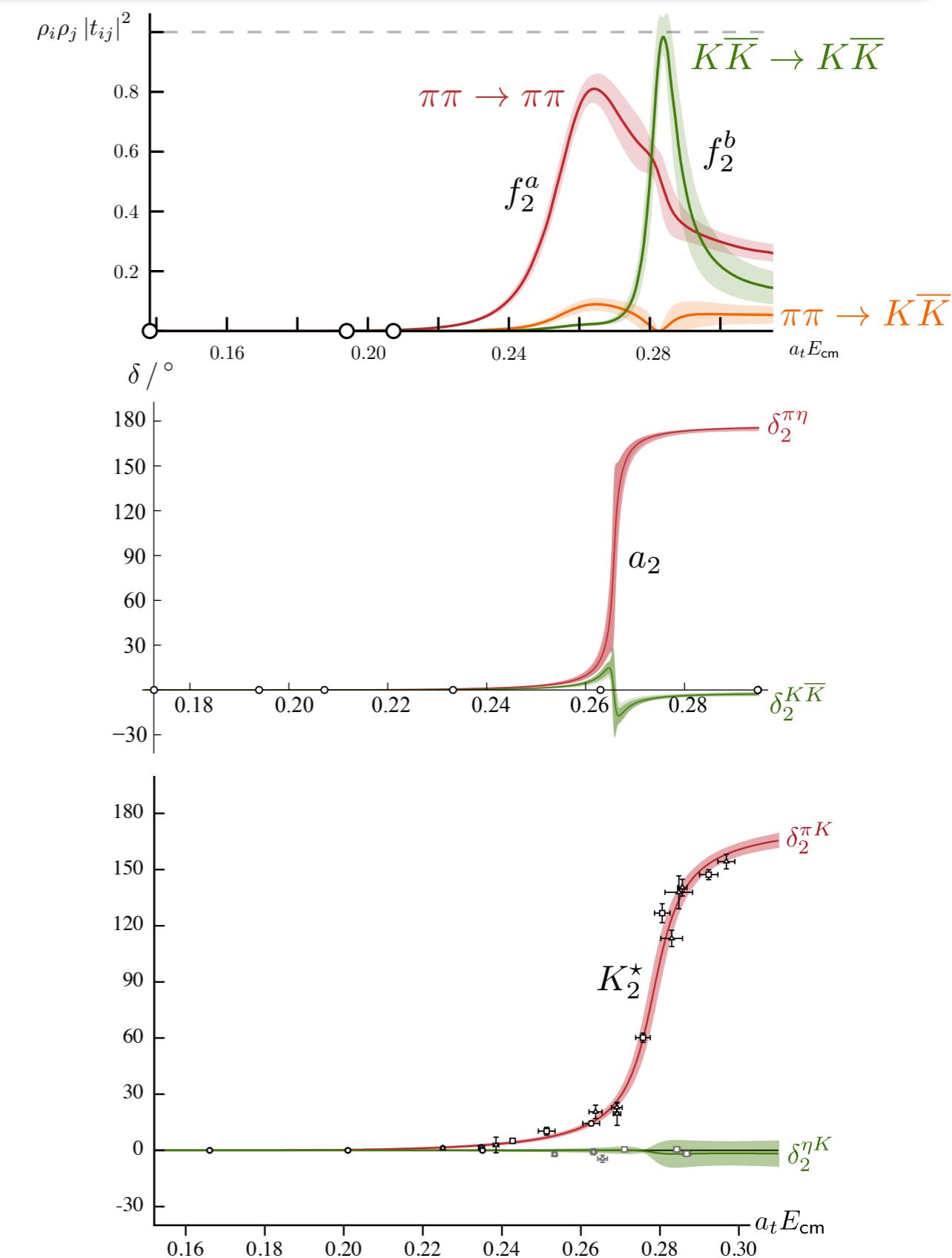
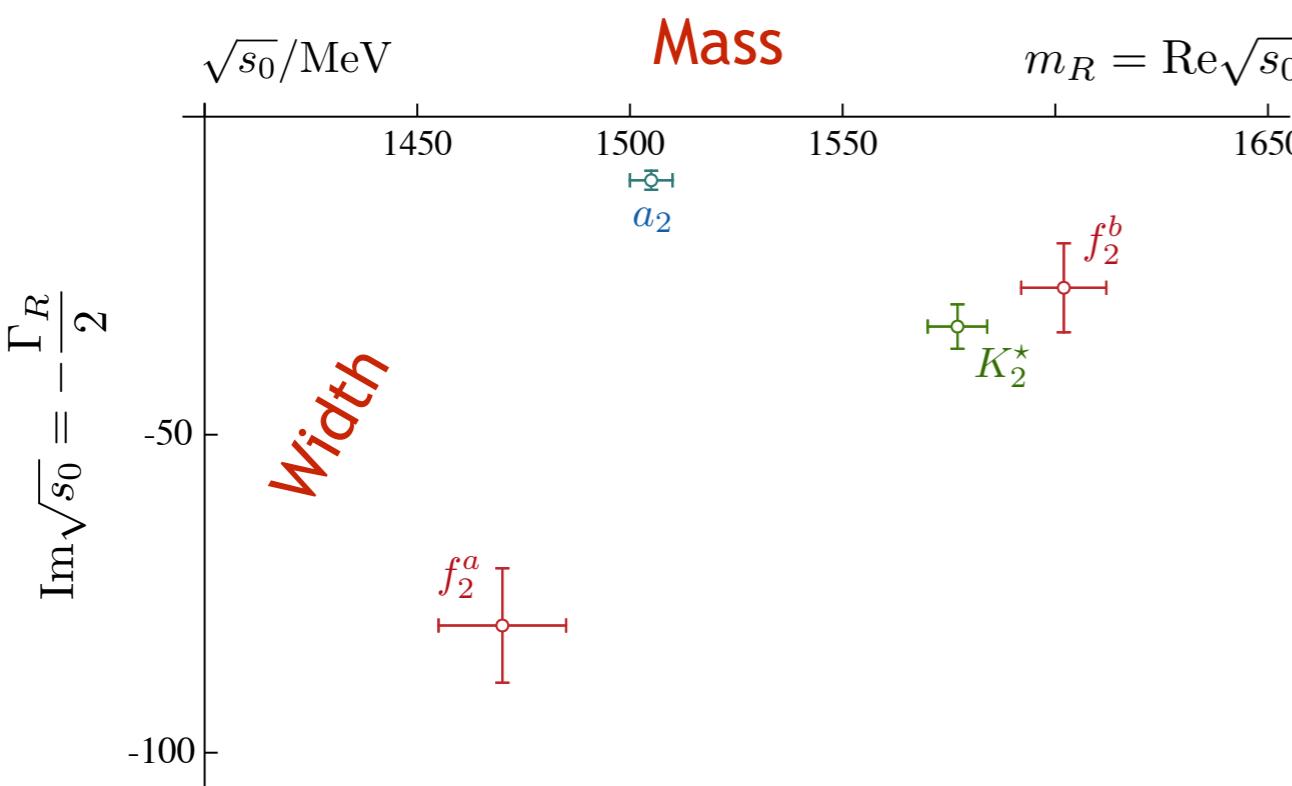
What does QCD have to say?

# Lightest tensors at $m_\pi=391$ MeV

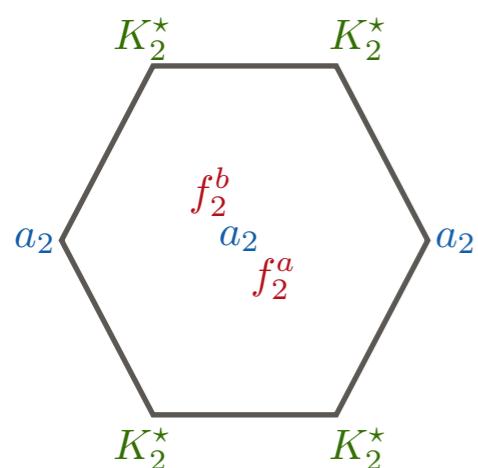
PRD97, 054513 (2018)



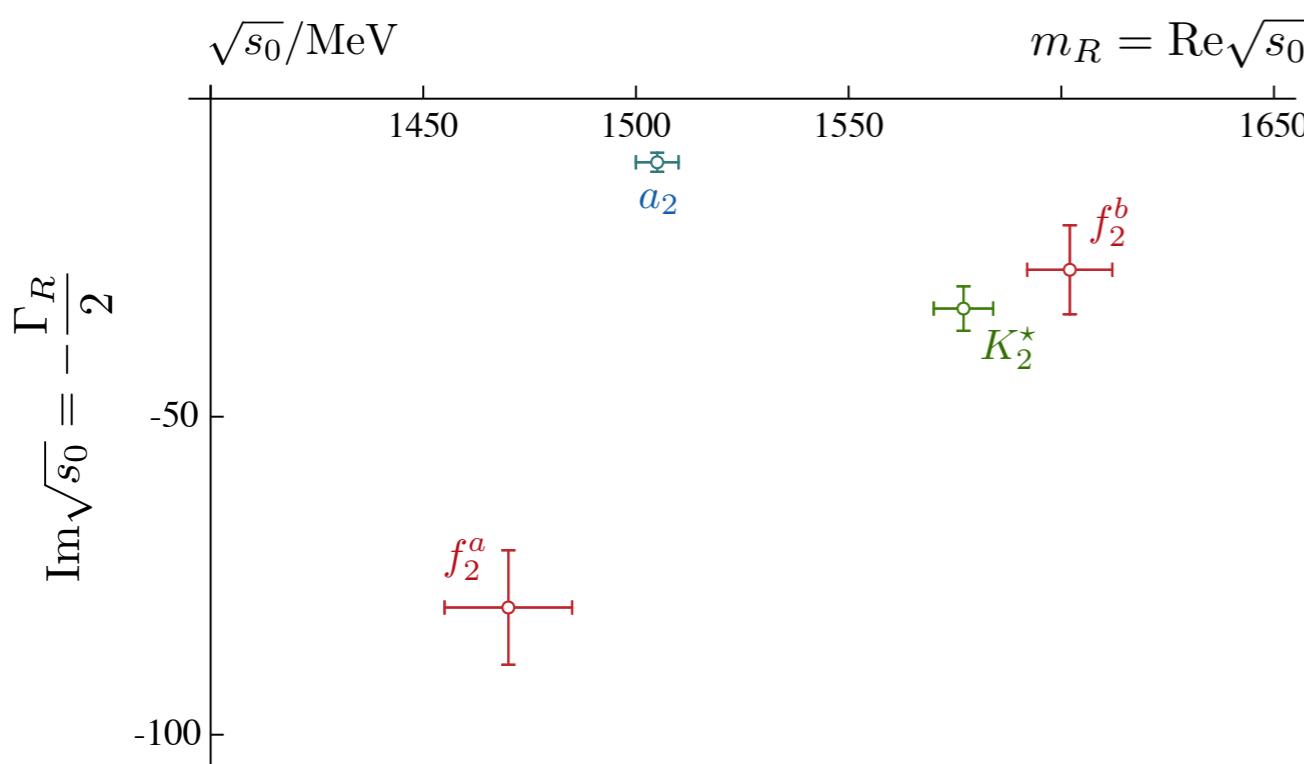
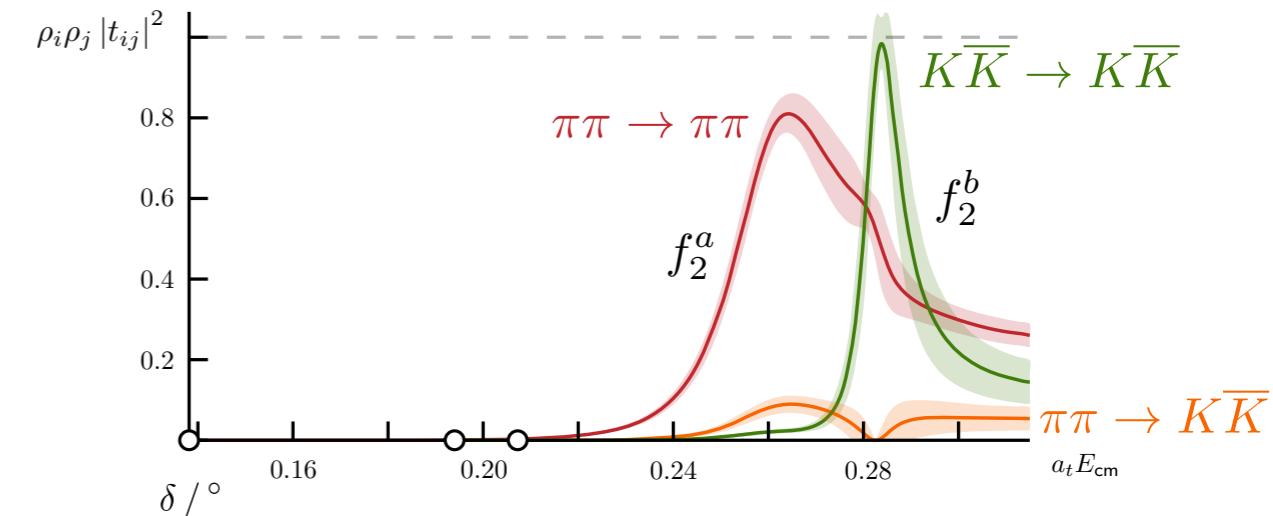
spin = 2



# Lightest tensors at $m_\pi=391$ MeV



spin = 2

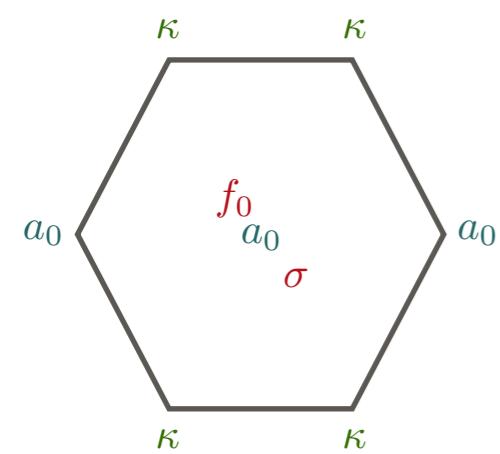


Used as motivation in  
GlueX detector upgrade proposal

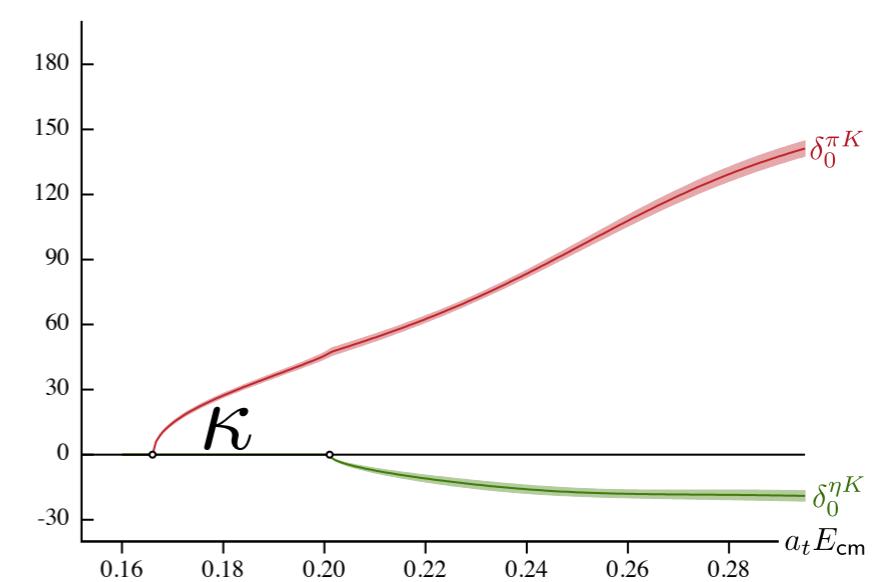
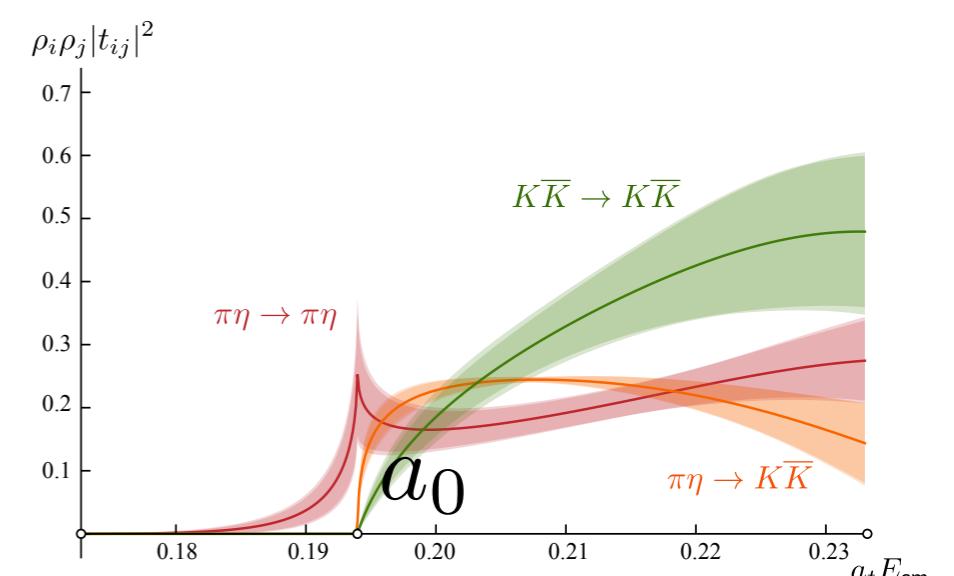
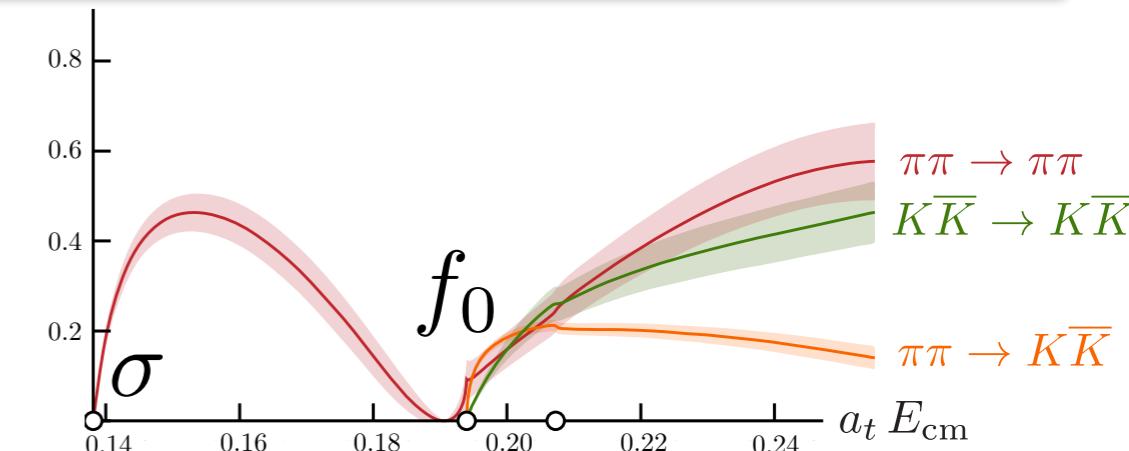
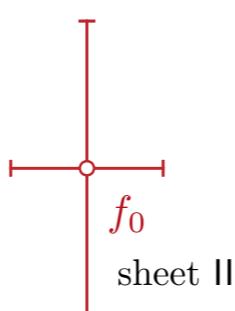
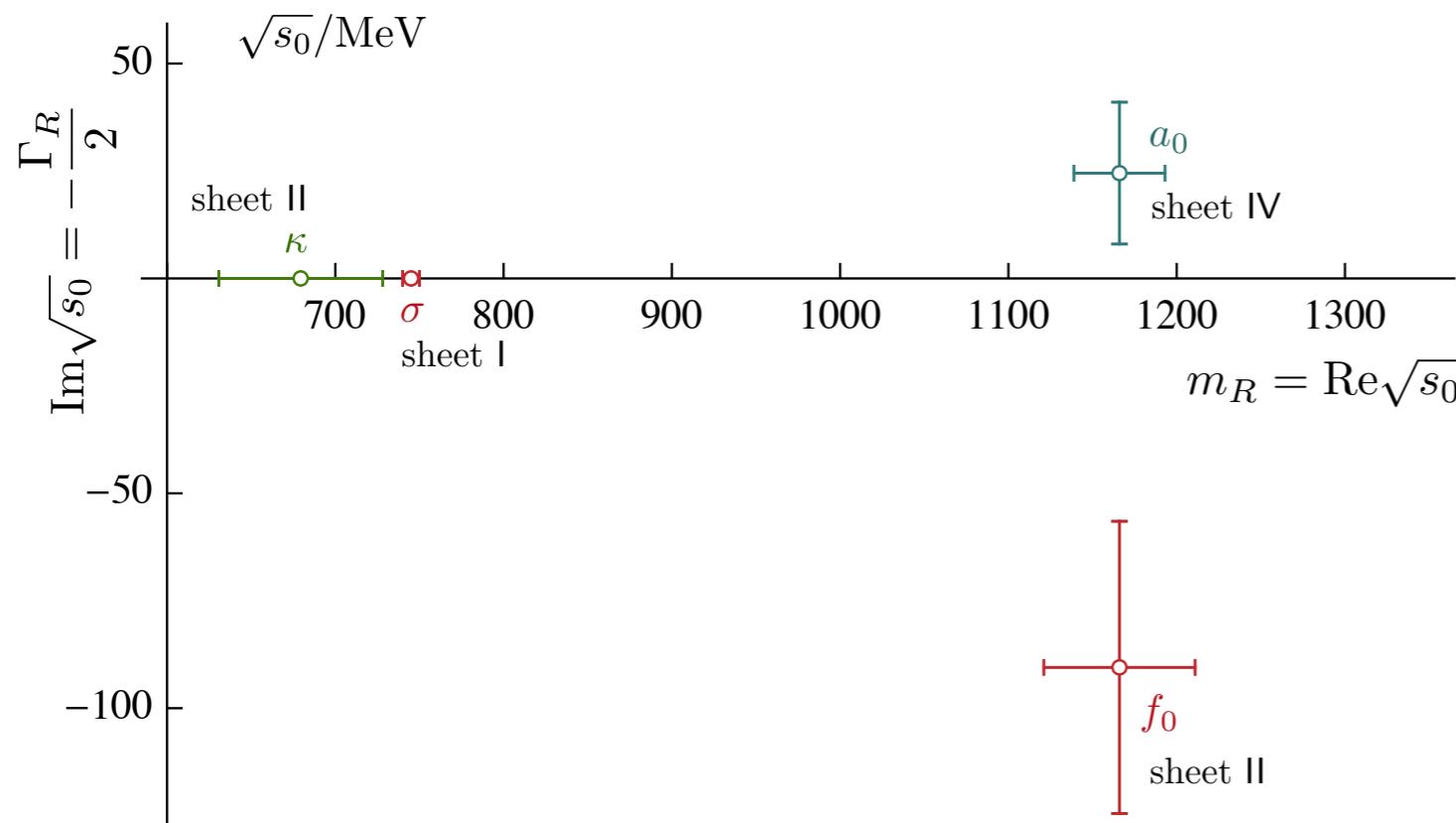
# Lightest scalars at $m_\pi=391$ MeV



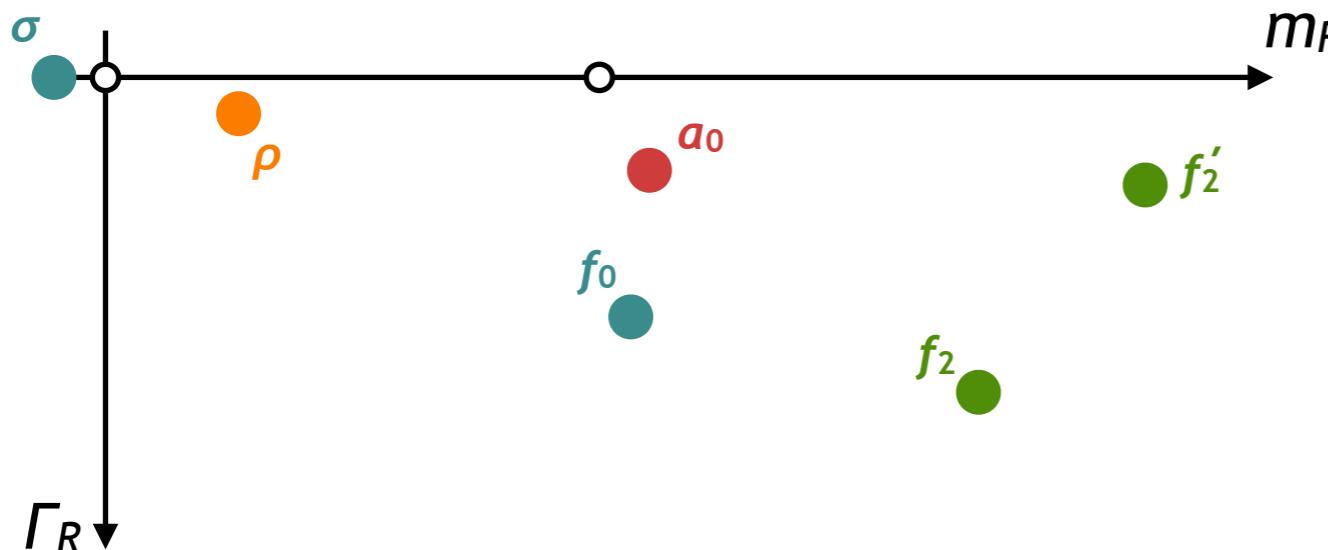
HadSpec: Phys.Rev.D97 (2018);  
Phys.Rev.Lett.118 (2017)



spin = 0



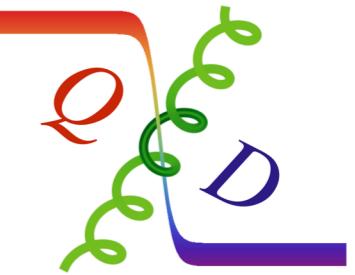
# Light meson resonances at $m_\pi \sim 391$ MeV



Have found the nonets of spin = 0, 1, 2 from QCD

Thanks to SciDAC

# Anatomy of the Proton Mass



- Your mass comes from  $M = E/c^2$  of the nucleons inside your atoms.

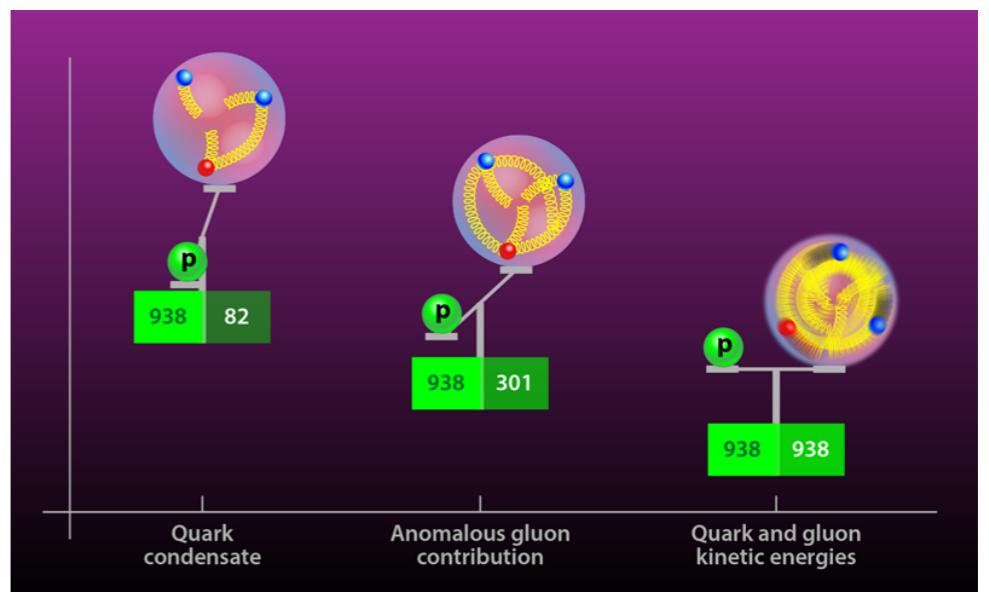
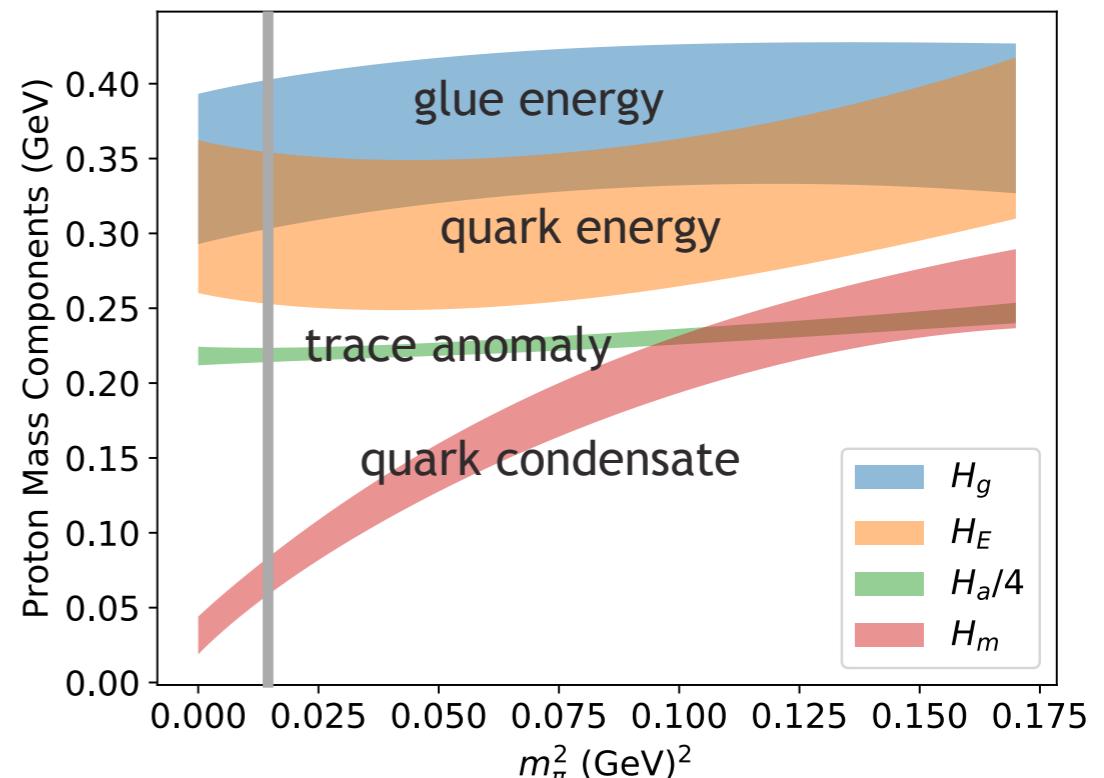
- The energy comes from:

- quark masses (Higgs-Yukawa);
- dimensional transmutation;
- quark and gluon kinetic energies.

- Yang *et al.* ( $\chi$ QCD), [Phys.Rev.Lett 121 \(2018\)](#).

- [ScienceNews!](#)

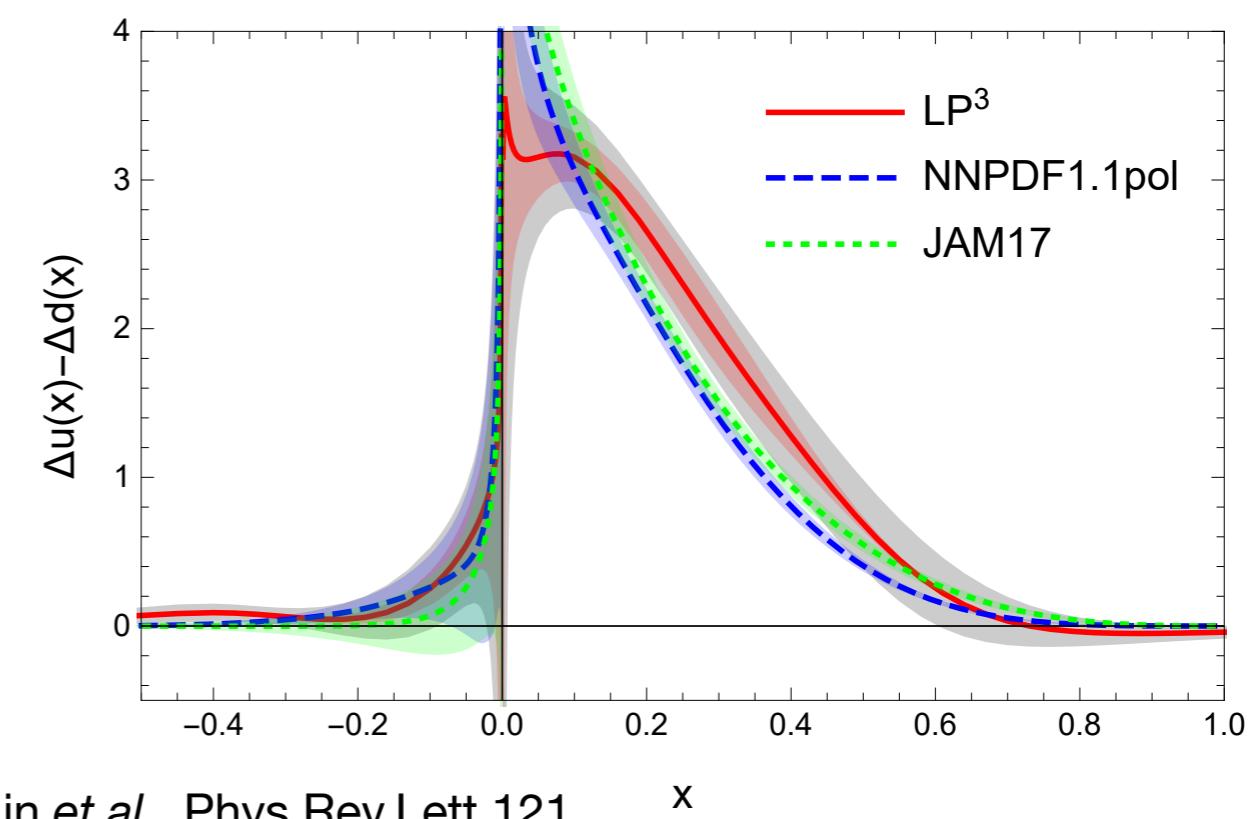
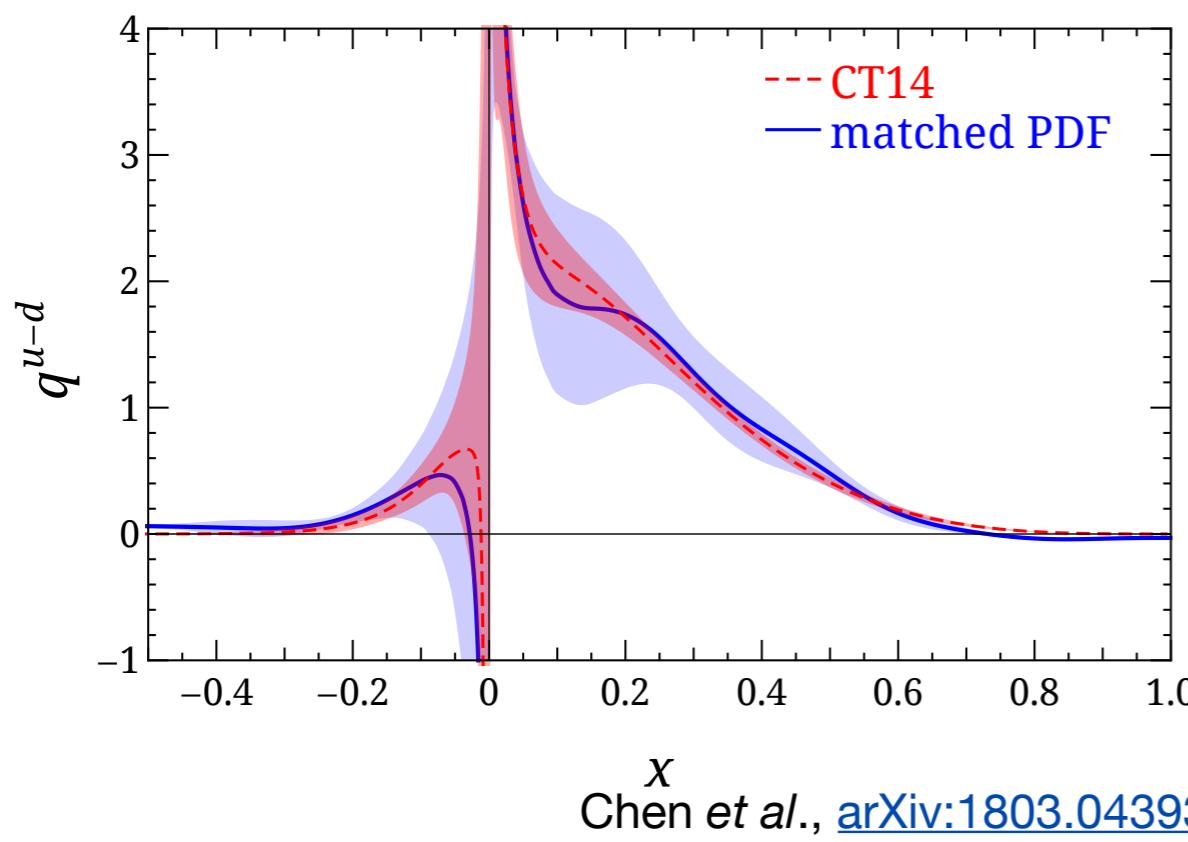
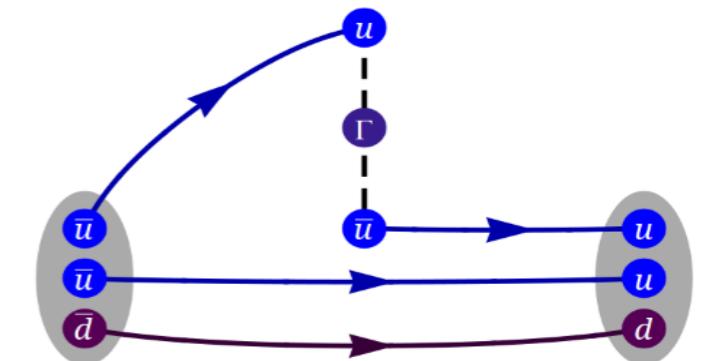
[APS Physics!](#) ➡



# Parton Distribution Functions

- Any improvement benefits **LHC searches**.
- Key measure of nucleon structure.
- Explosion of numerical & theoretical work  $\Leftarrow$  first USQCD studies.

X. Ji, [Phys.Rev.Lett 110 \(2013\)](#)

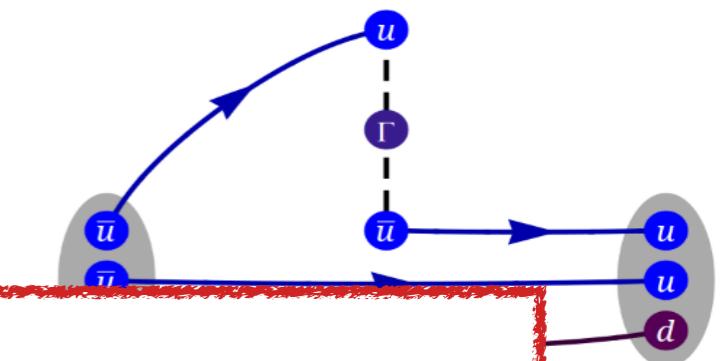


Chen et al., [arXiv:1803.04393](#); Lin et al., Phys.Rev.Lett 121

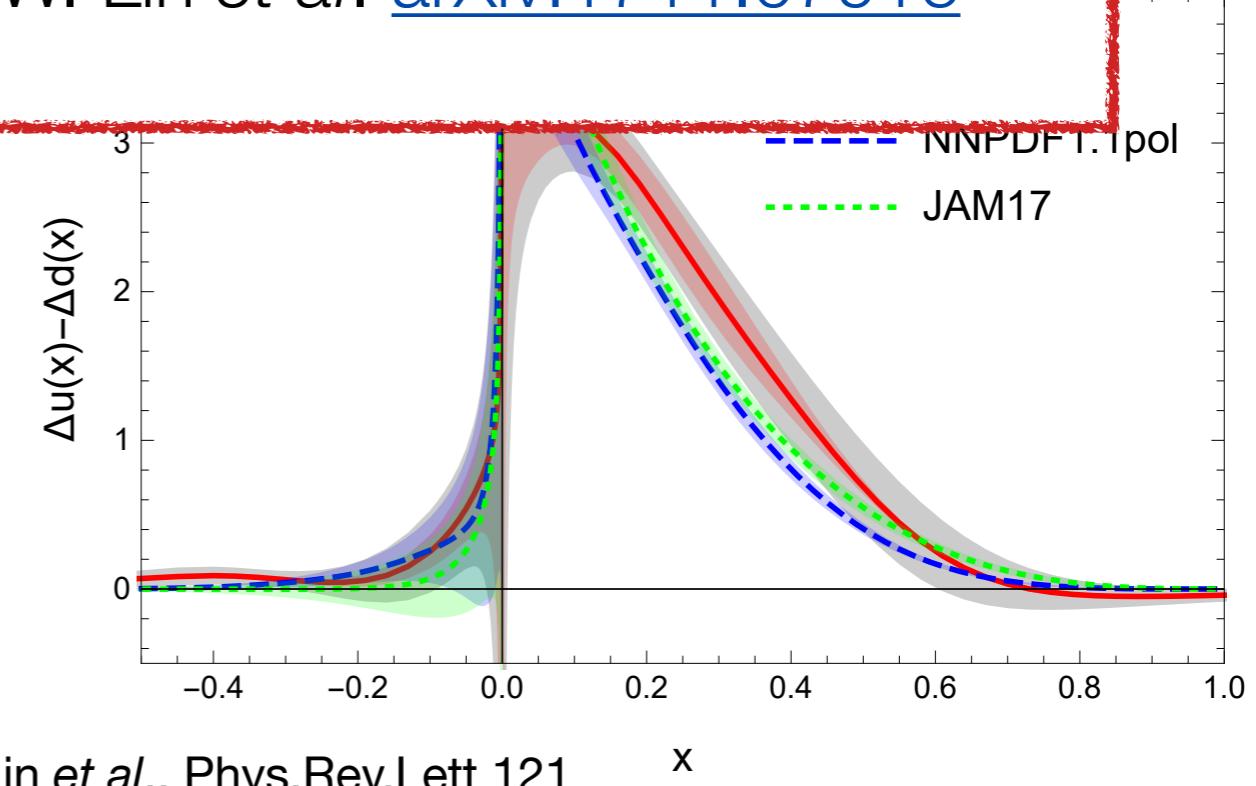
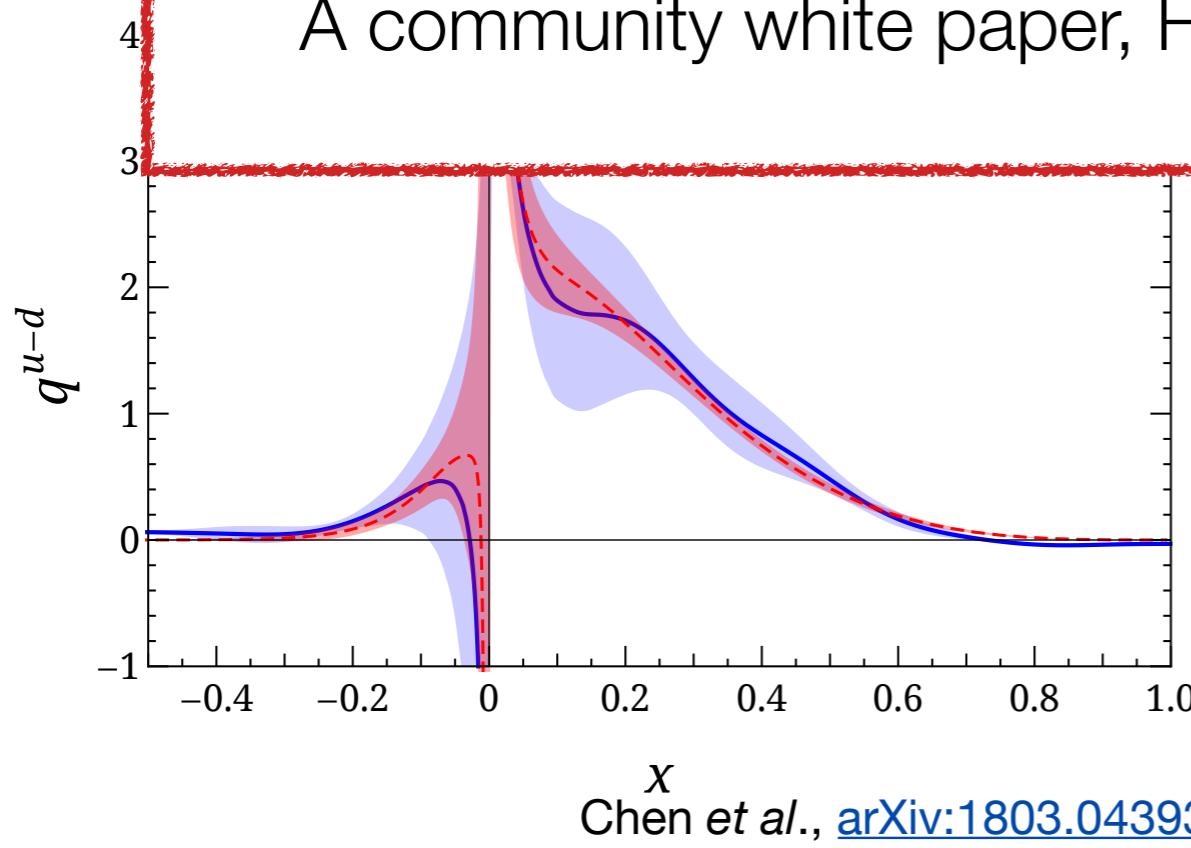
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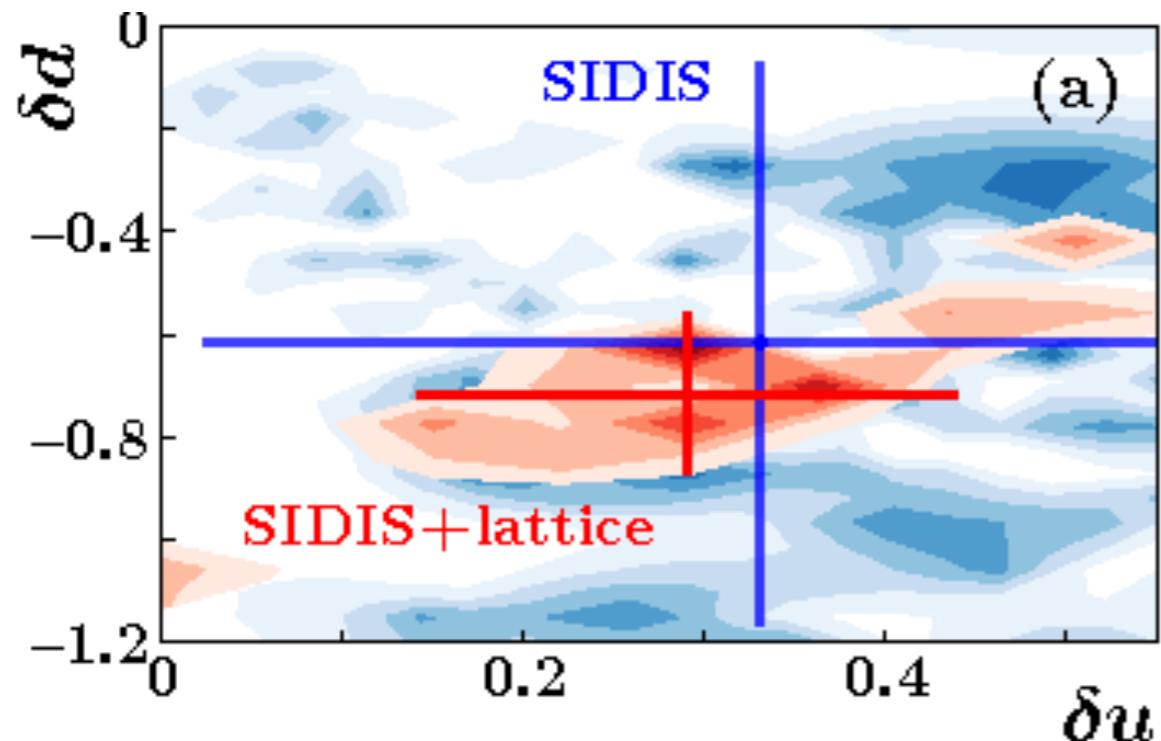
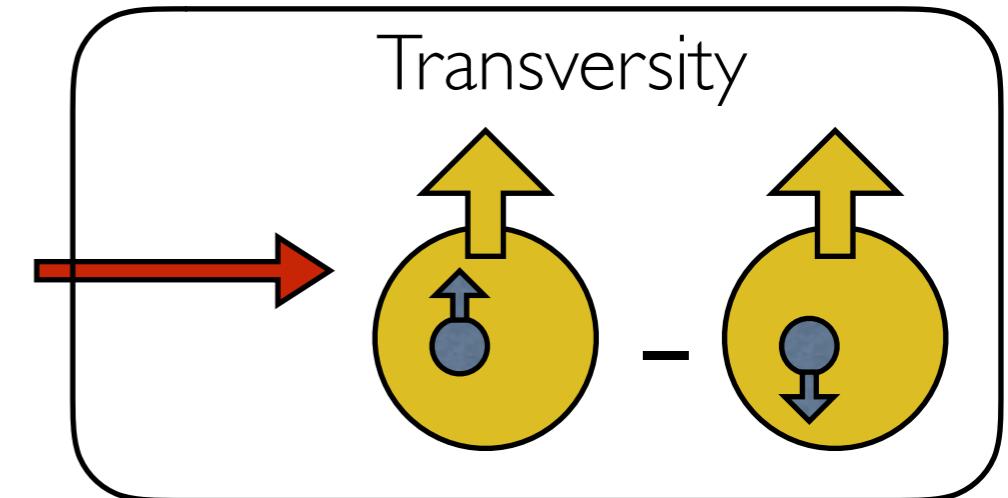
Parton distributions and lattice QCD calculations:  
A community white paper, H.-W. Lin *et al.* [arXiv:1711.07916](#)



Chen *et al.*, [arXiv:1803.04393](#); Lin *et al.*, Phys.Rev.Lett 121

# Nucleon Structure

- Quark transverse parton distribution:
  - aligned vs. anti-aligned in polarized target;
  - poorly determined in semi-inclusive DIS.



- ← New global analysis including lattice-QCD constraints:
- [Lin, et.al., Phys.Rev.Lett 120 \(2018\)](#)
  - Lattice QCD can contribute in many areas of nucleon structure.

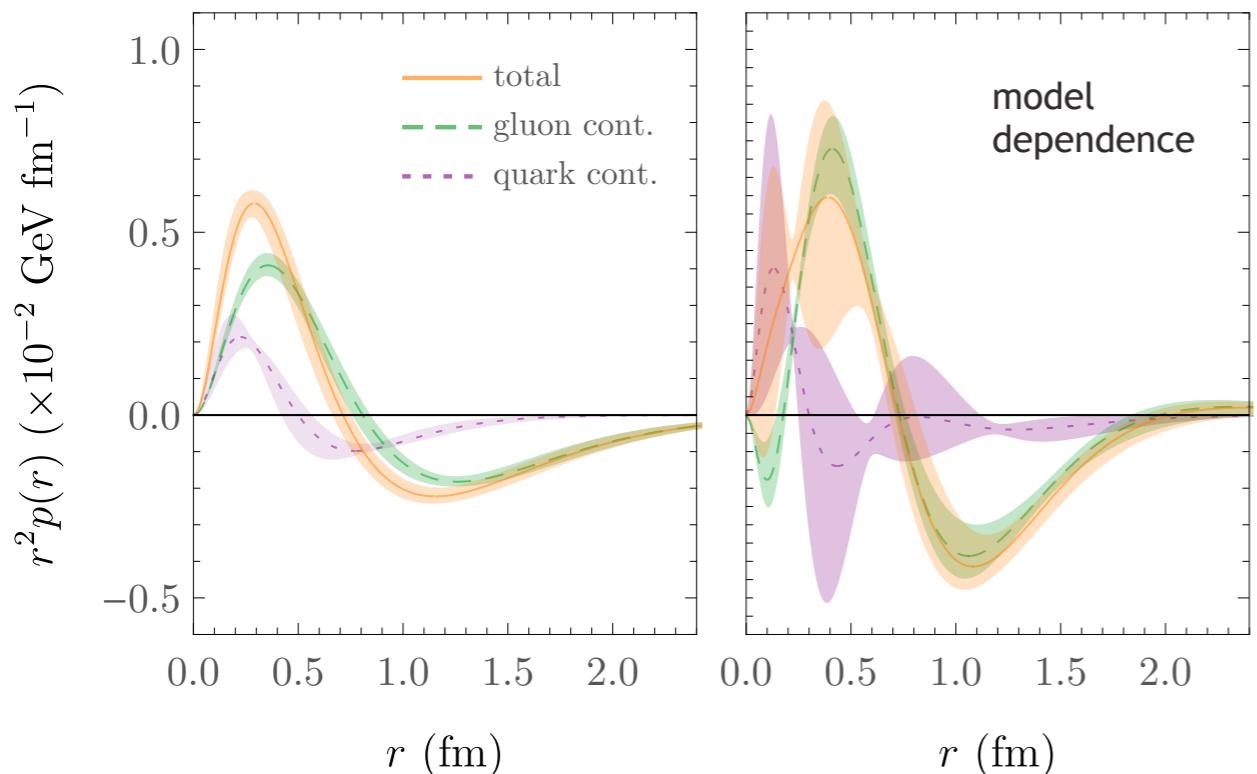
# Pressure in the proton

Pressure of quark/glue mapped in expt.

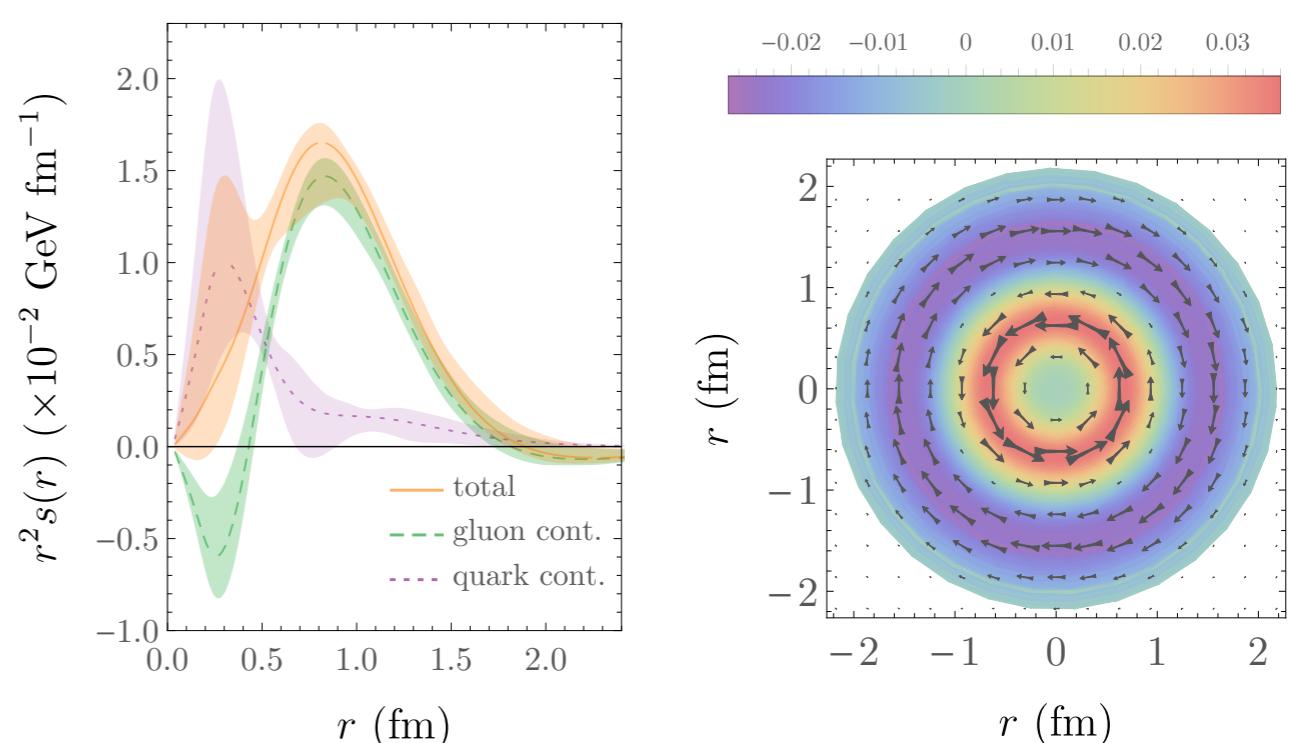
LQCD can compute Energy-Mom. Tensor matrix elements



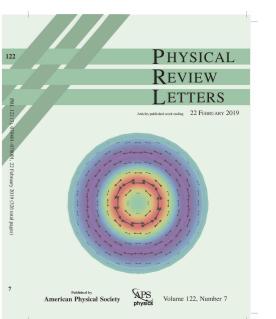
$r^2 * \text{pressure}$



$r^2 * \text{shear}$



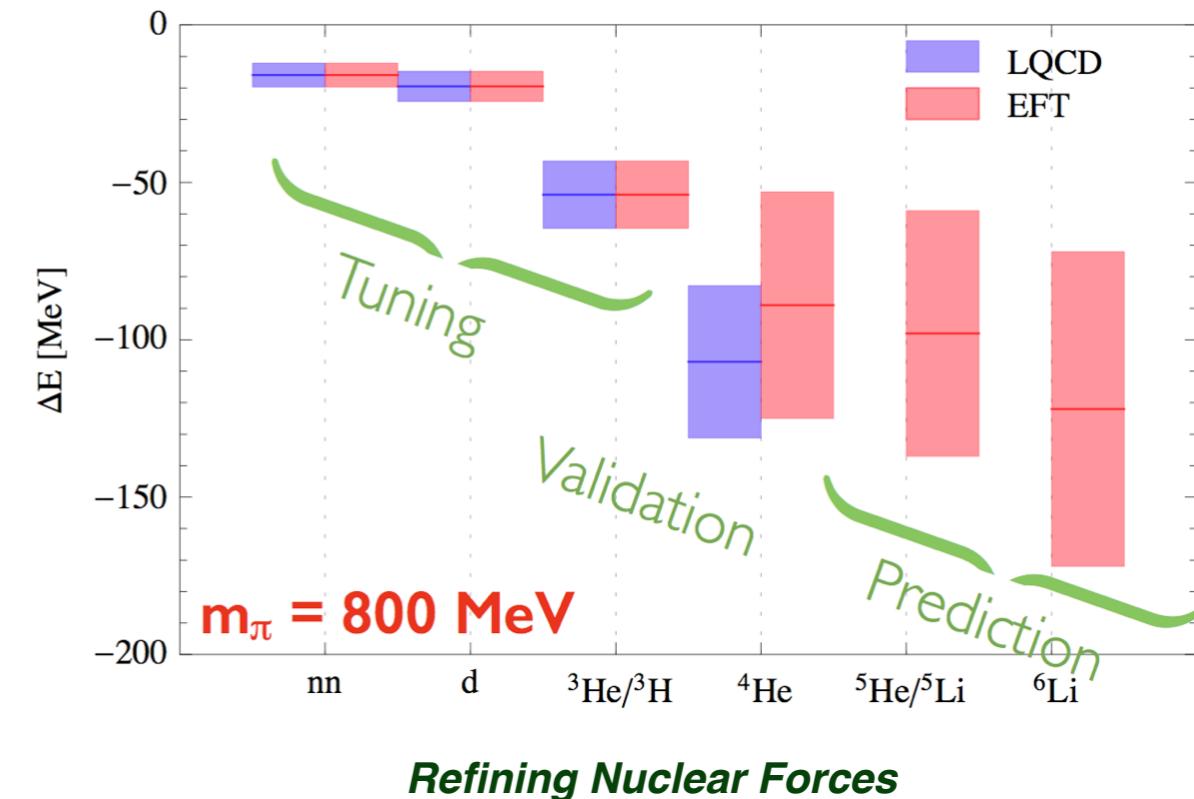
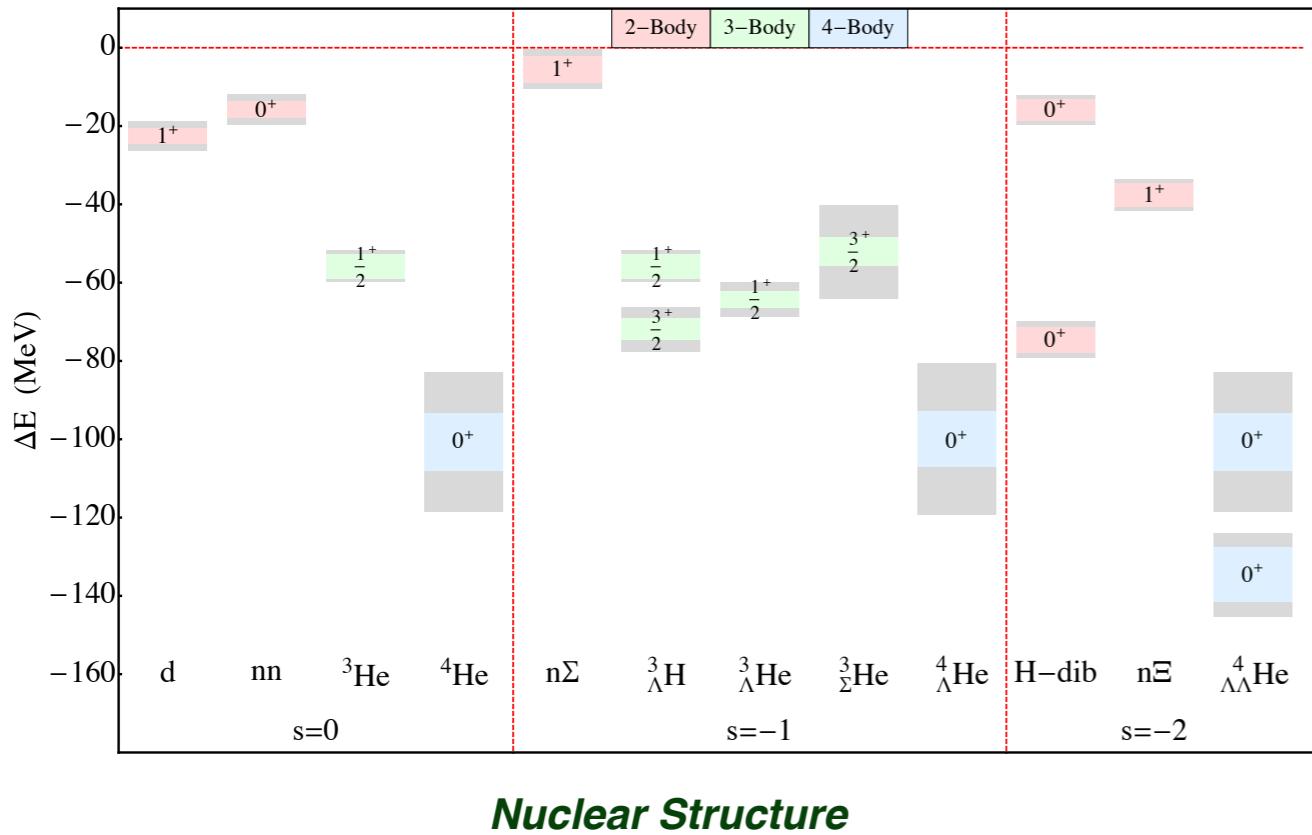
quarks/glue repulsive at core; attractive at boundary  
glue lurks near boundary



PRL122, 072003 (2019)

# QCD for nuclei - milestone

The binding energies of light nuclei+strange nuclei



"Effective field theory for lattice nuclei",  
PRL 114 052501 (2015)

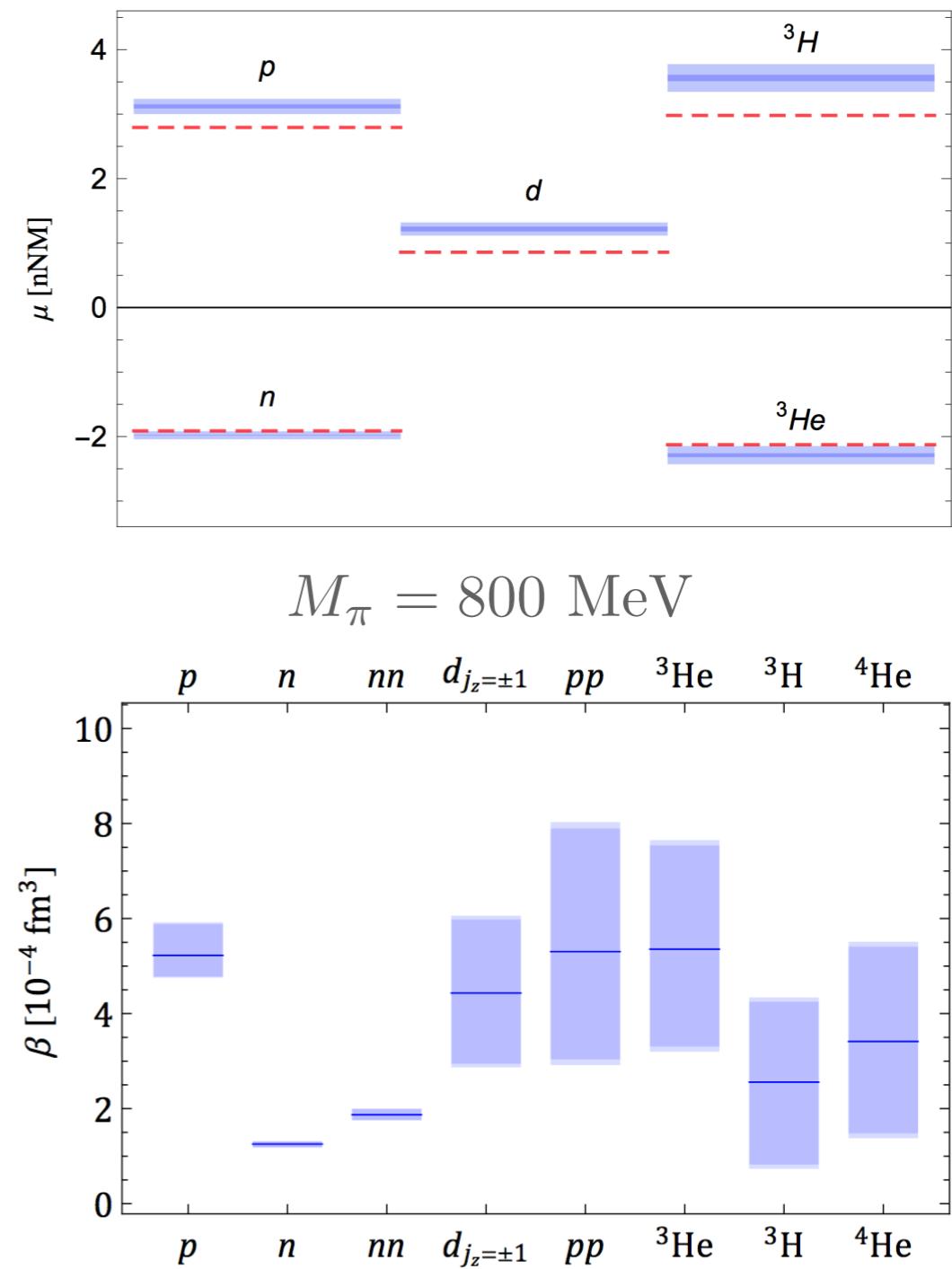
- First calculations of binding energies of light hypernuclei
- QCD calculations used to validate and predict properties of nuclei

'Light nuclei and hyper nuclei from QCD  
in the limit of SU(3) flavor symmetry'  
PRD 87 034506 (2013)



# Light Nuclei

- Nuclear structure offers new insights and challenges, e.g.:
  - parton distributions  $\longleftrightarrow$  EMC effect.
- First steps: isovector magnetic moments and polarizabilities up to  $A = 4$ .
- Striking agreement with experiment even at unphysical light-quark mass.
- New directions: first computations of weak decays with  $A \leq 3$ .
  - $g_A$  quenching
  - pp fusion
  - Double  $\beta\beta$  decay

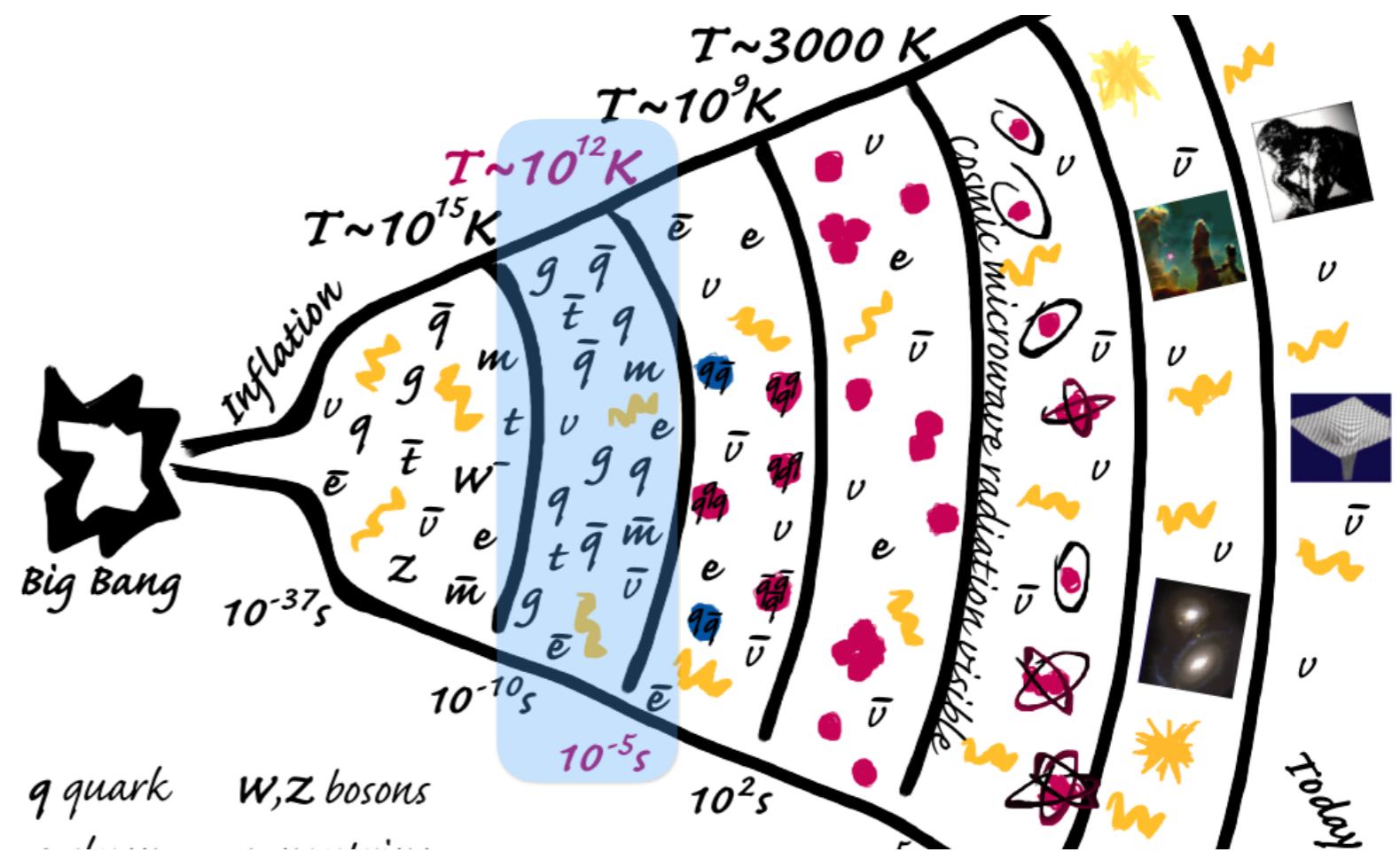
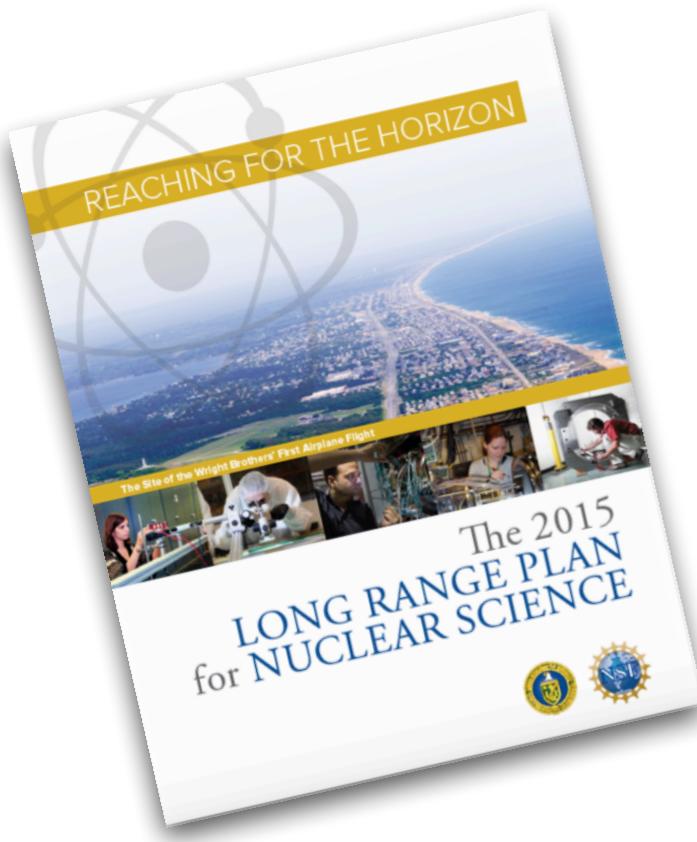


Beane, et al., [Phys.Rev.Lett.113 \(2014\)](#); Tiburzi, et al., [Phys.Rev.D96 \(2017\)](#)

# Hot-Dense matter

properties of quark gluon plasma (QGP)

the big questions ...

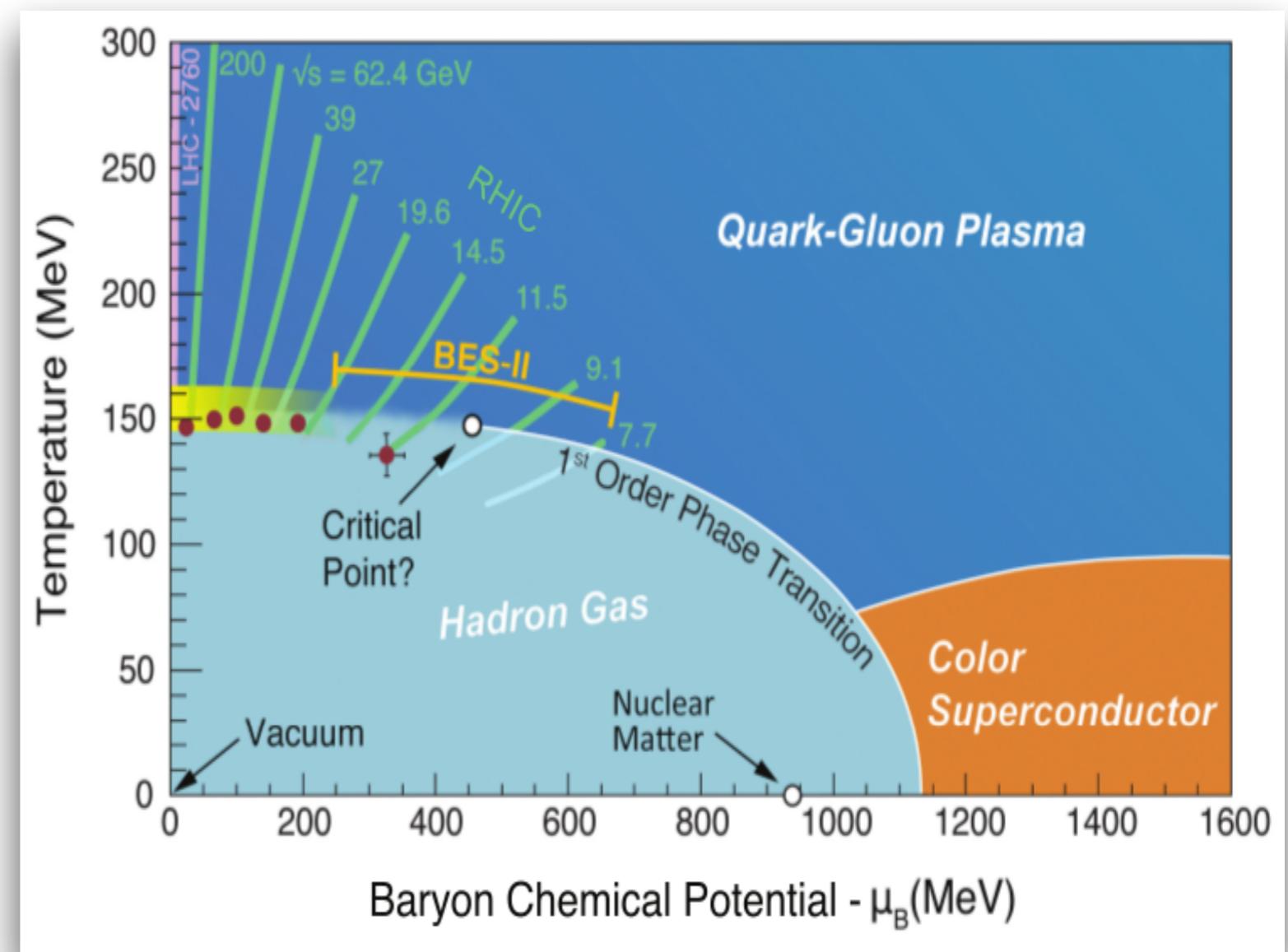
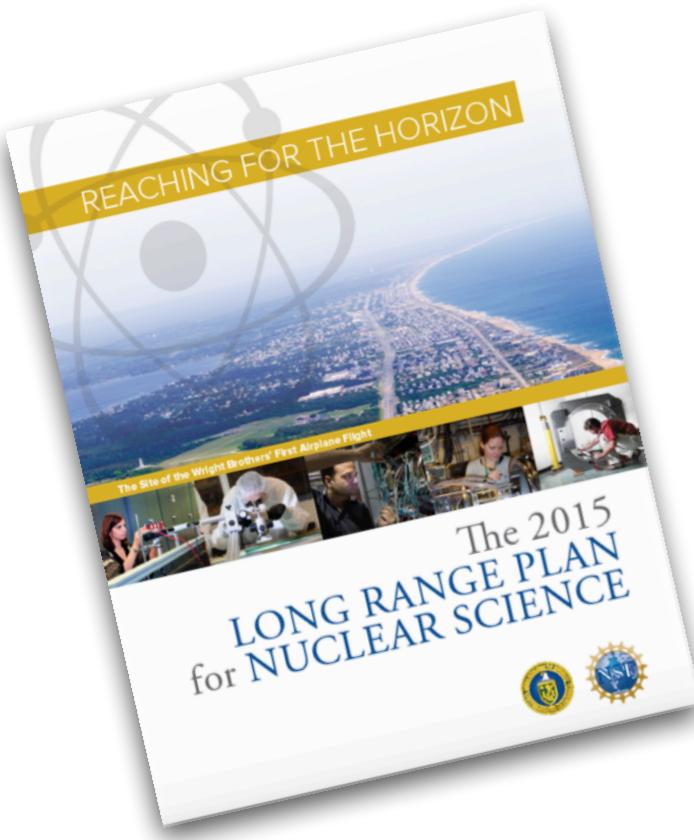


characterize the matter that existed  
~ micro-seconds after the Big Bang

# Hot-Dense matter

properties of strongly interacting matter

the big questions ...



- varying temperatures and densities

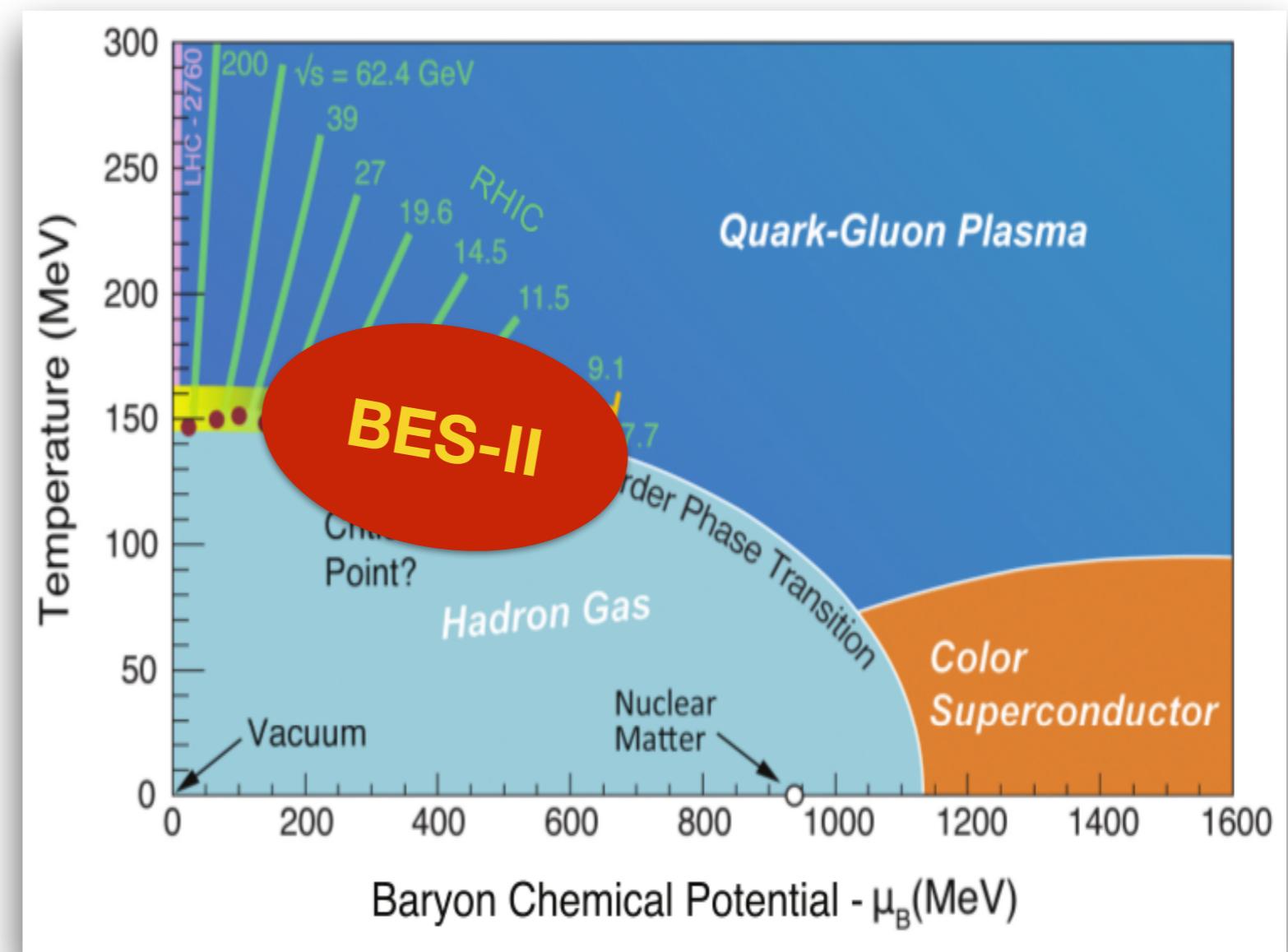
# Hot-Dense matter - new expt. at BNL

Beam Energy Scan-II @ RHIC



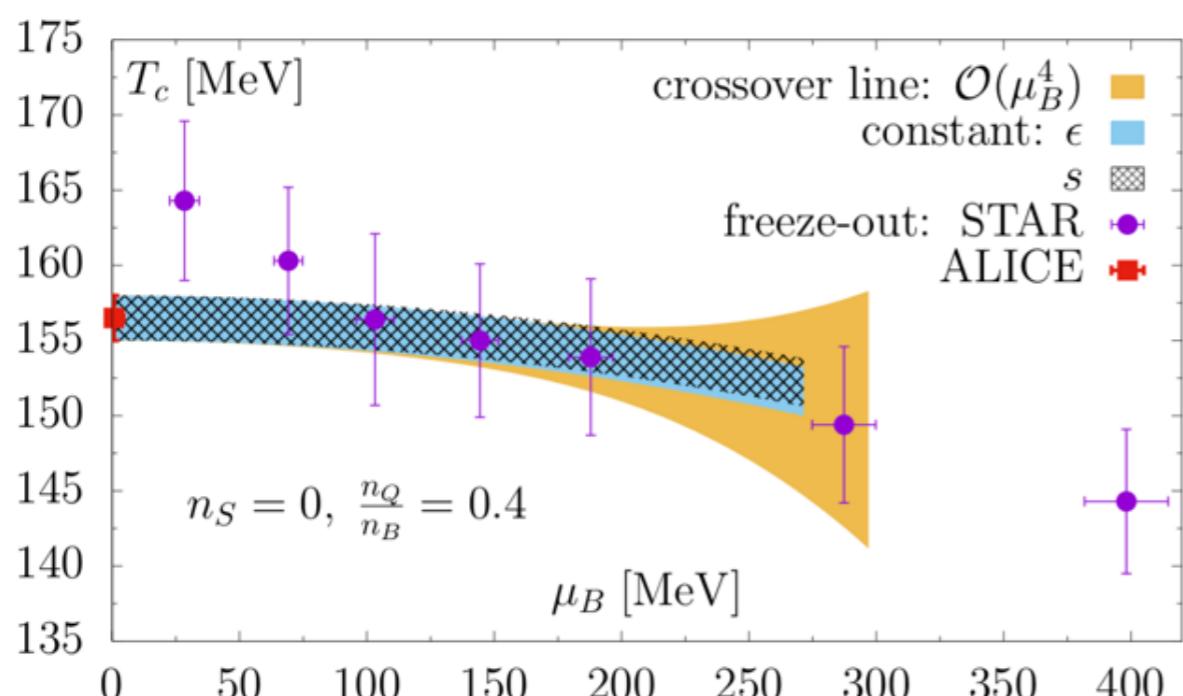
2019-2021

Phase diagram? Critical point?

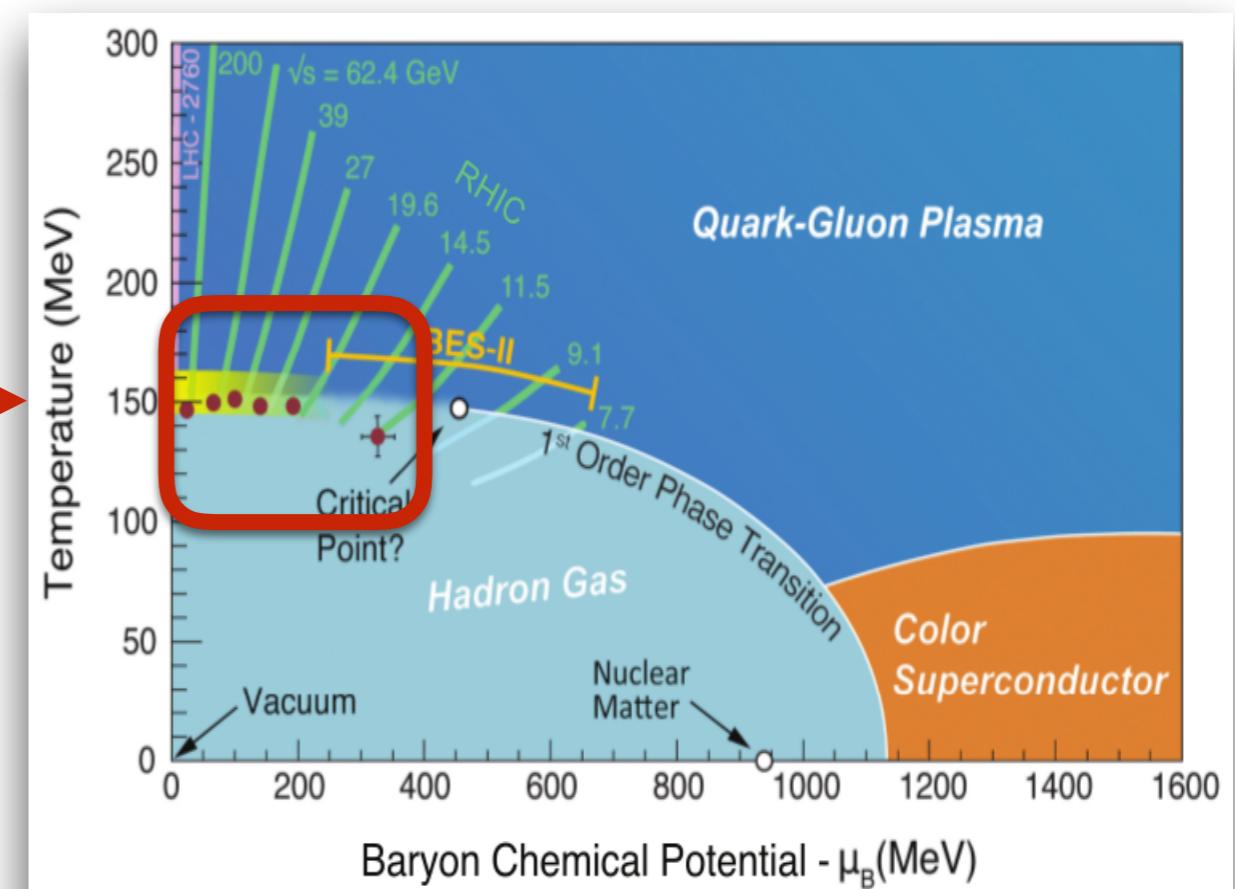


# QCD phase boundary computed

LQCD calculation



Guide for BES-II program



- Chemical freeze-out
  - in vicinity of QCD phase boundary
  - coincides with lines of constant energy & entropy density

Phys. Lett. B795 (2019)

# Computational Requirements

## Gauge generation

- Leadership level
- Strong scaling



## Analysis

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



## Strong scaling limited

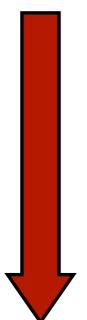
- Comms/compute less balanced in recent machines
- Latency in comms important
- Require comms reduced linear solvers
- 1-flavor solvers

Symplectic PDE integrators

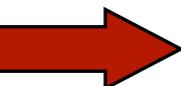
Data-parallel code gen. with comms

## Throughput challenge

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

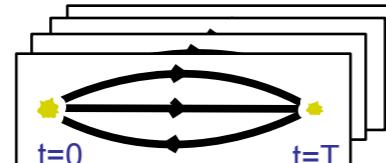


## Contractions



## Correlators

- $O(1M)/cfg$

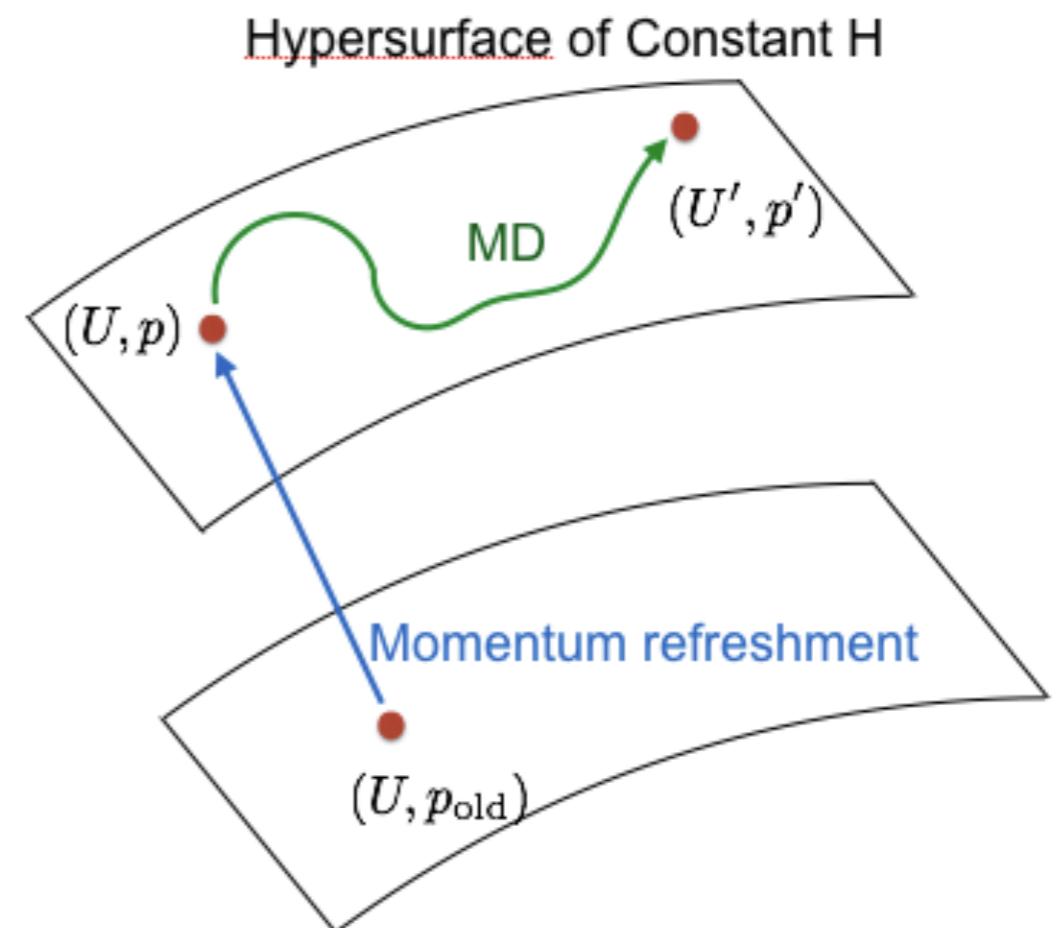


## “Workflow” challenge

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

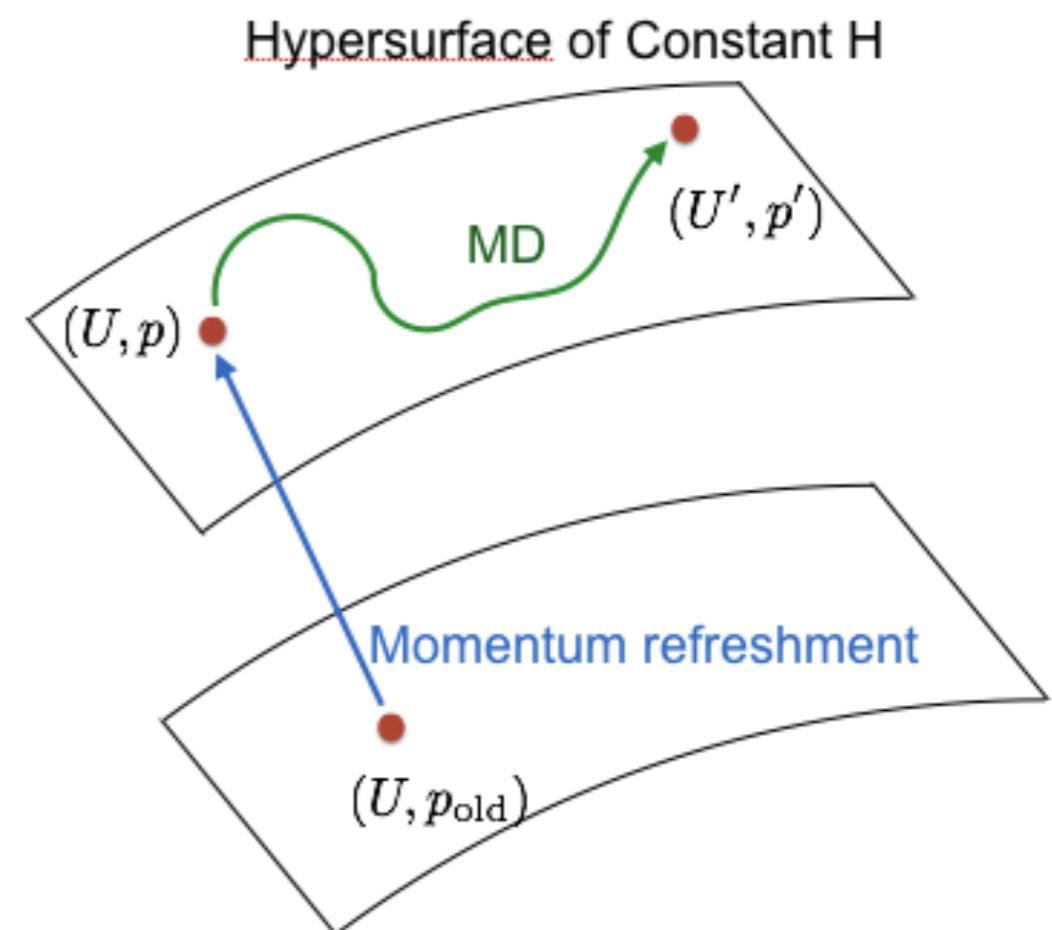
# How to produce gauge fields?

- Hamilton's equations - 1<sup>st</sup> order coupled differential eqns.
- Each integration step: sparse matrix solution
- Strong scaling challenge
- Limitations



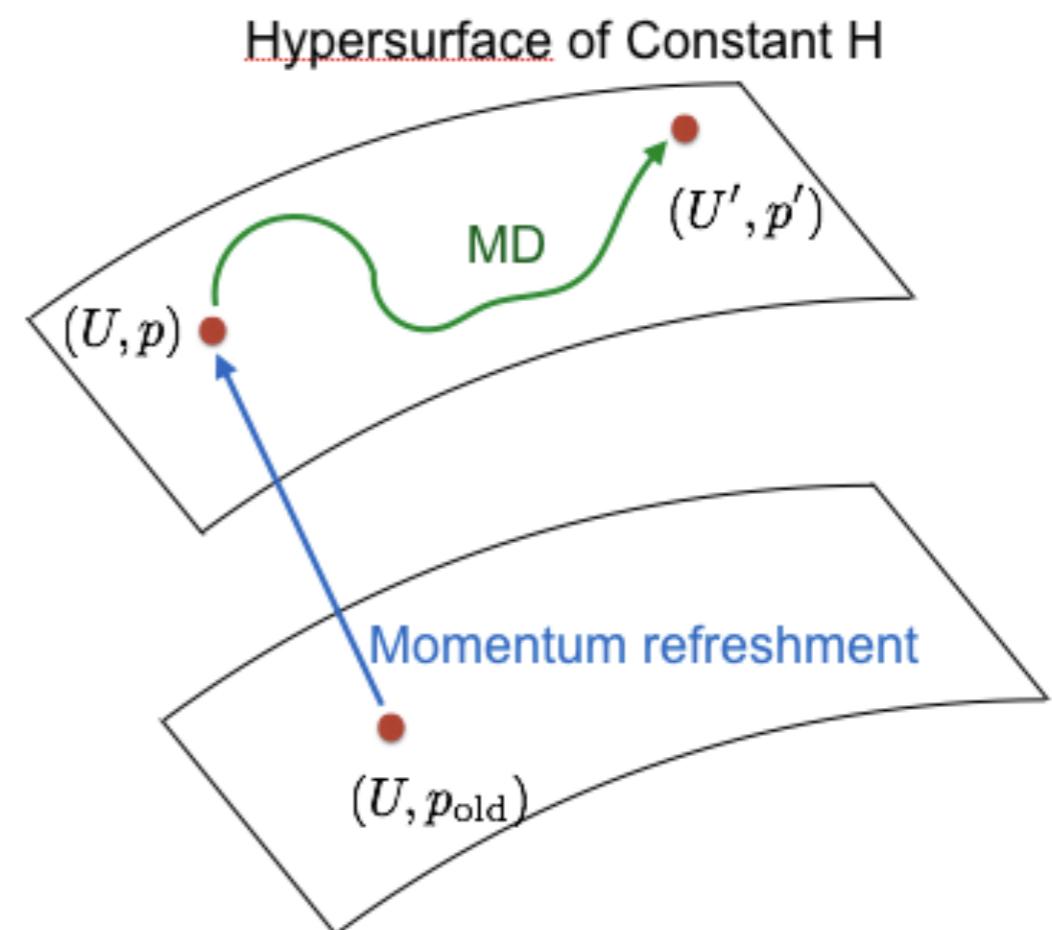
# How to produce gauge fields?

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  - Each integration step: sparse matrix solution
  - Strong scaling challenge
- 
- Limitations
    - Must be “reversible”



# How to produce gauge fields?

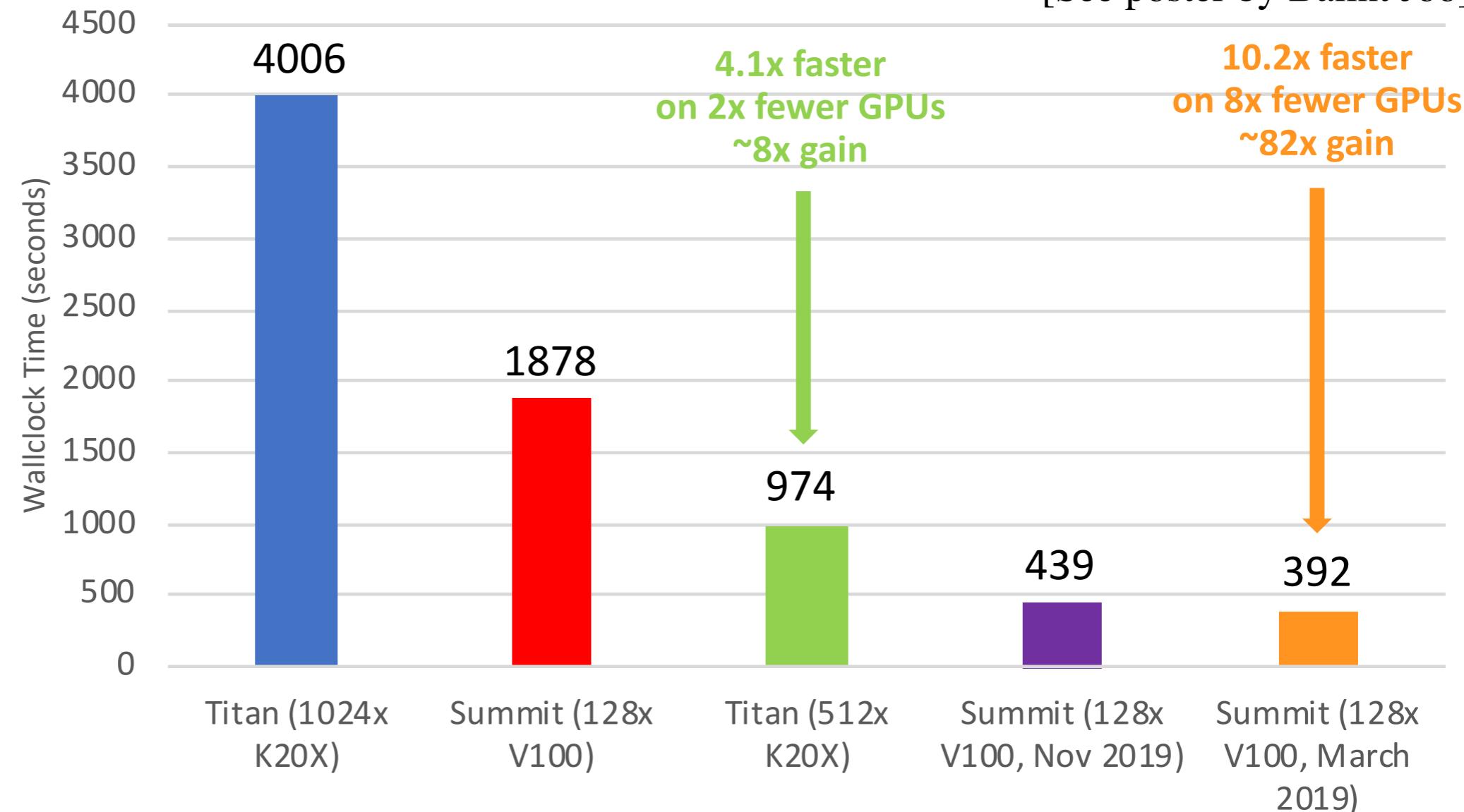
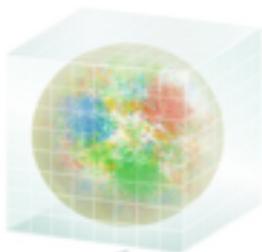
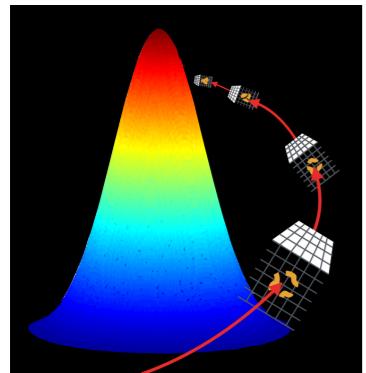
- Hamilton's equations - 1<sup>st</sup> order coupled differential eqns.
- Each integration step: sparse matrix solution
- Strong scaling challenge
- Limitations
  - Must be “reversible”
  - No adaptive time steps



# Accelerating QCD gauge generation on GPUs

Collaboration involving ASCR support and Industry partners

[See poster by Balint Joo]



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

# Next: Improved “throughput”

## Gauge generation

- Leadership level
- Strong scaling



## Analysis

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

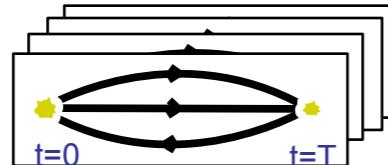


## Contractions



## Correlators

- $O(1M)/cfg$



## Strong scaling limited

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

Symplectic PDE integrators

Data-parallel code gen. with comms

## Throughput challenge

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

## “Workflow” challenge

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

# Accelerating propagators

[See poster by Balint Joo]

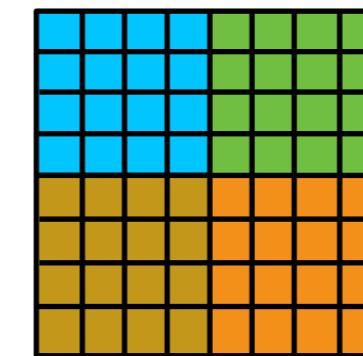
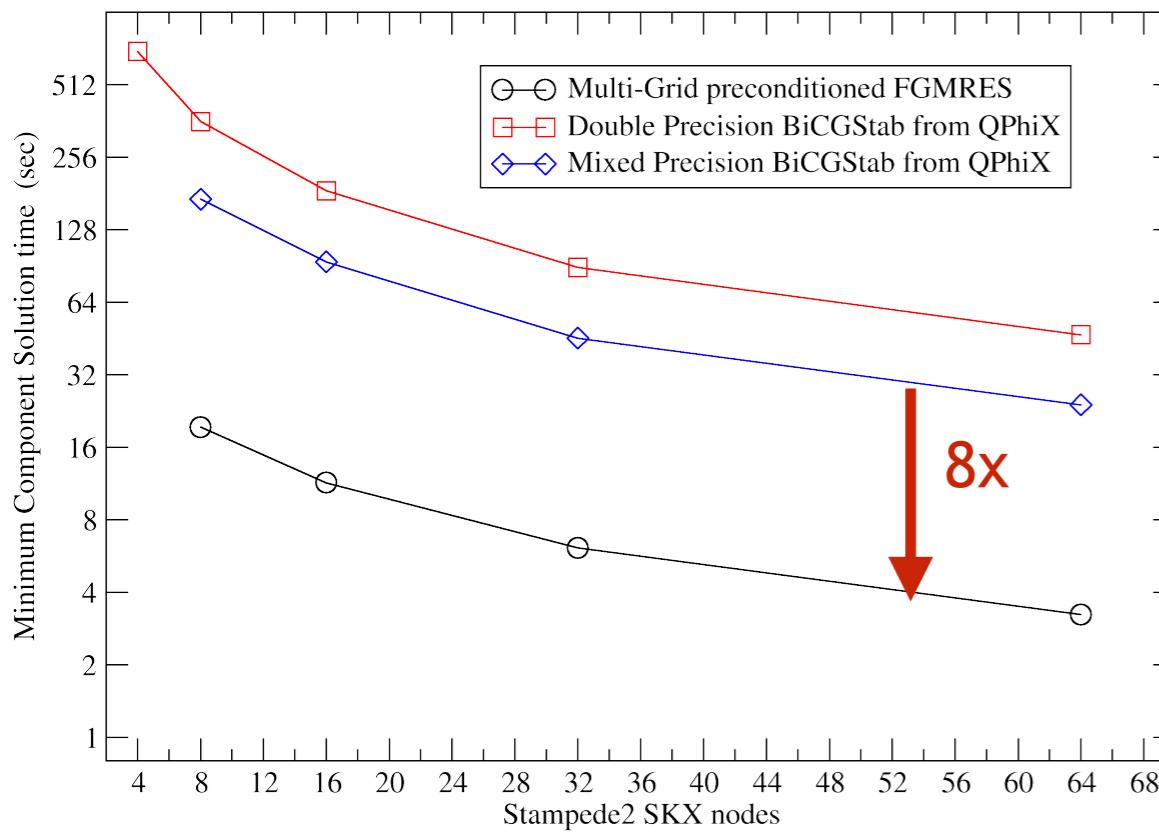
Collaboration involving ASCR support and Industry partners

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

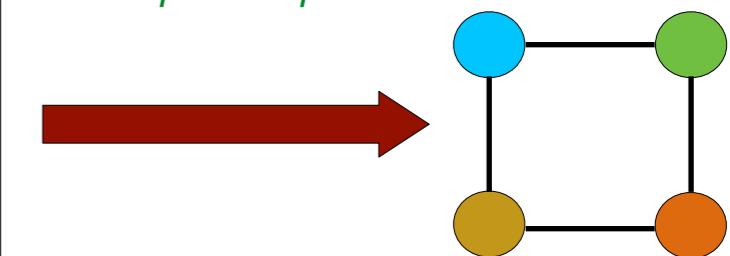
Stampede 2 (Skylake) - Strong scaling

Performance similar on KNL systems

$V=64^3 \times 128$  lattice,  $m_\pi \sim 172$  MeV,  $a=0.092$  fm



Restriction: Aggregation over sites, colors, chiral spin components.



- Issues: AVX512, nested parallelism for aggregation
- 8x speedup over conventional methods

Happy times on Cori-KNL

# Reducing contraction/correlator costs

## Gauge generation

- Leadership level
- Strong scaling



## Analysis

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



## Strong scaling limited

- Comms/compute less balanced in recent machines
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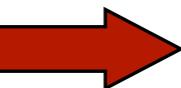
Symplectic PDE integrators

Data-parallel code gen. with comms

## Throughput challenge

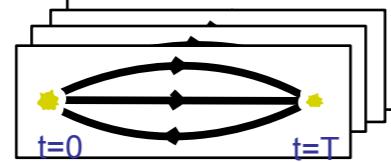
- Solvers still important
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## Contractions



## Correlators

- $O(1M)/cfg$



## “Workflow” challenge

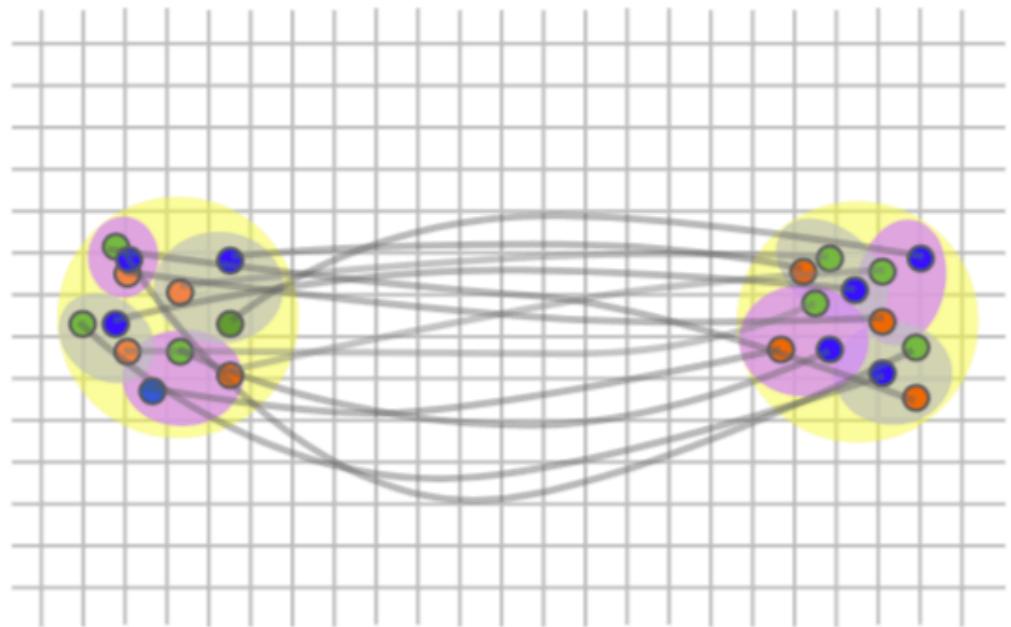
- Combinatorics -> improved graph theoretic methods
- Code generation for (sparse?) tensor contractions
- Job coordination -> Grid based

# QCD for nuclei

Collaboration involving ASCR support and Industry partners

- Quarks need to be tied together in all possible way

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

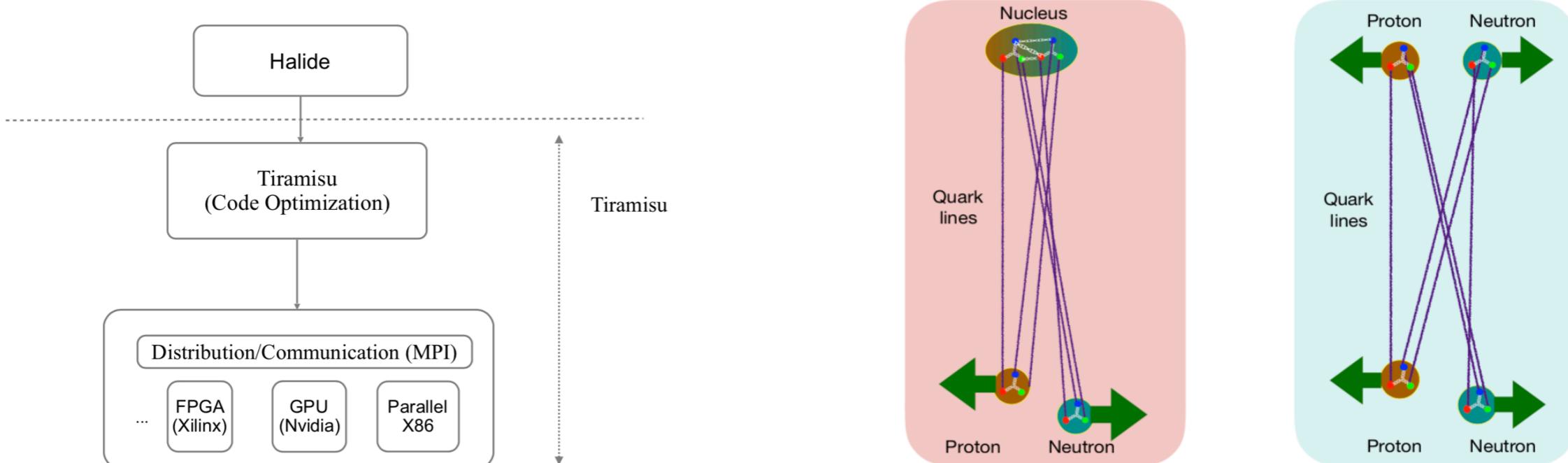


- Manage using algorithmic trickery - still significant graph contractions
- TACO @ MIT (cf TCE, Cyclops) <http://tensor-compiler.org>
  - general purpose tensor contraction compiler framework
  - target to QCD specific problems (sparsity patterns, ...)
  - Allow efficient exploration of methodology

# QCD for nuclei - Halide & Tiramisu

- Extend Tiramisu to accomodate LQCD & CUDA

[See poster session]



- 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

<http://tensor-compiler.org>

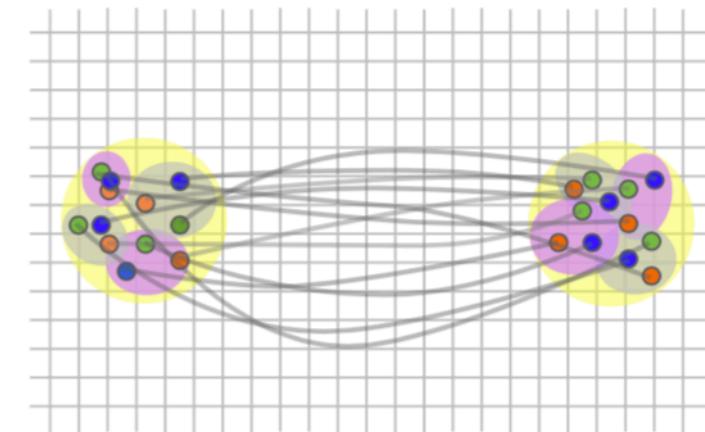
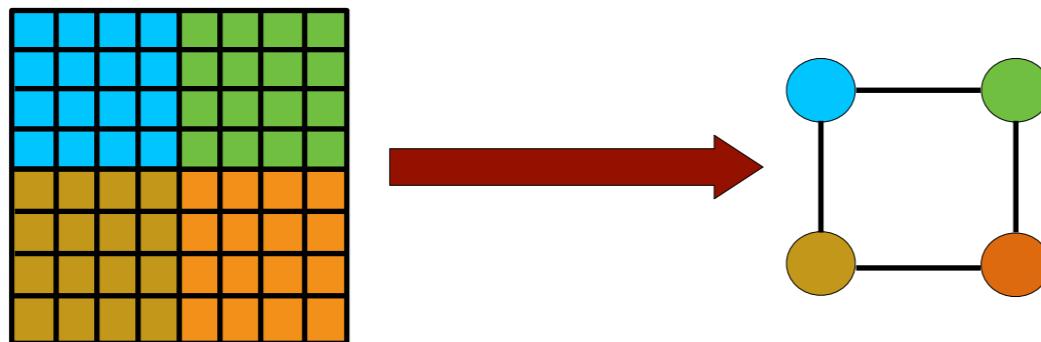
# QCD for nuclei - going to physic quark masses

- Reduce the volume scaling cost by reducing the volume!

[See poster session]

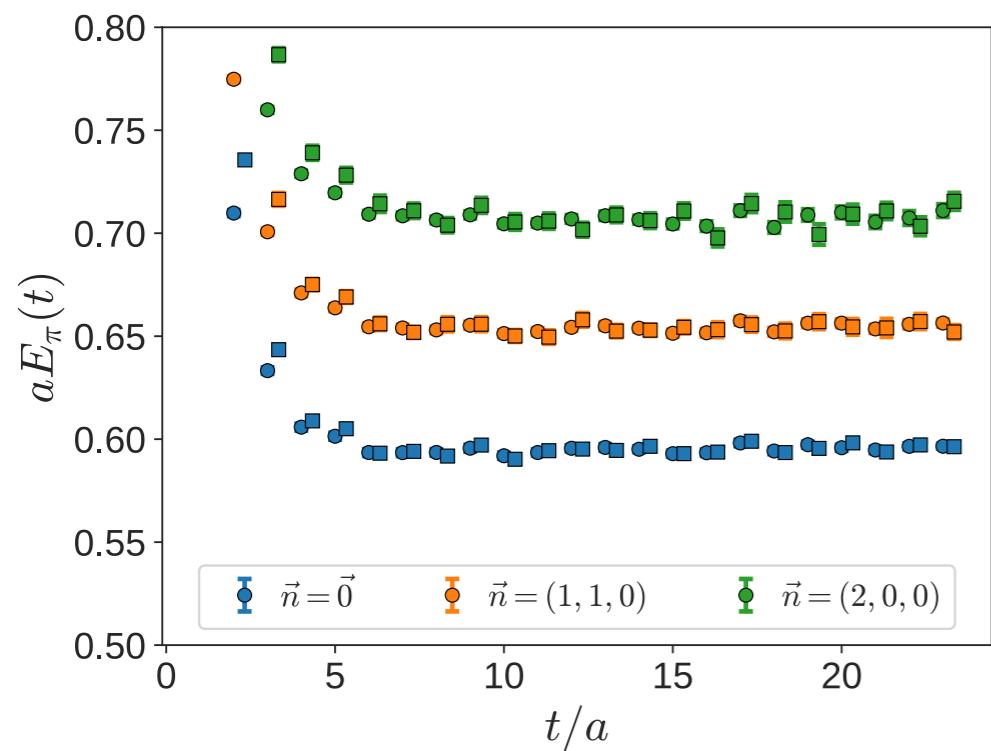
$$N_{\text{contractions}} = N_u! N_d! N_s! \quad (\sim 10^{1500} \text{ for } ^{208}\text{Pb})$$

Restriction: Aggregation over sites



- Combine with optimized block constructions → substantially reduces cost

Correlation function



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

Calculations in progress for nuclei

# SciDAC-4 is a partnership

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- 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