Lattice Quantum Chromodynamics Project

SciDAC-4

Robert Edwards
Jefferson Lab

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

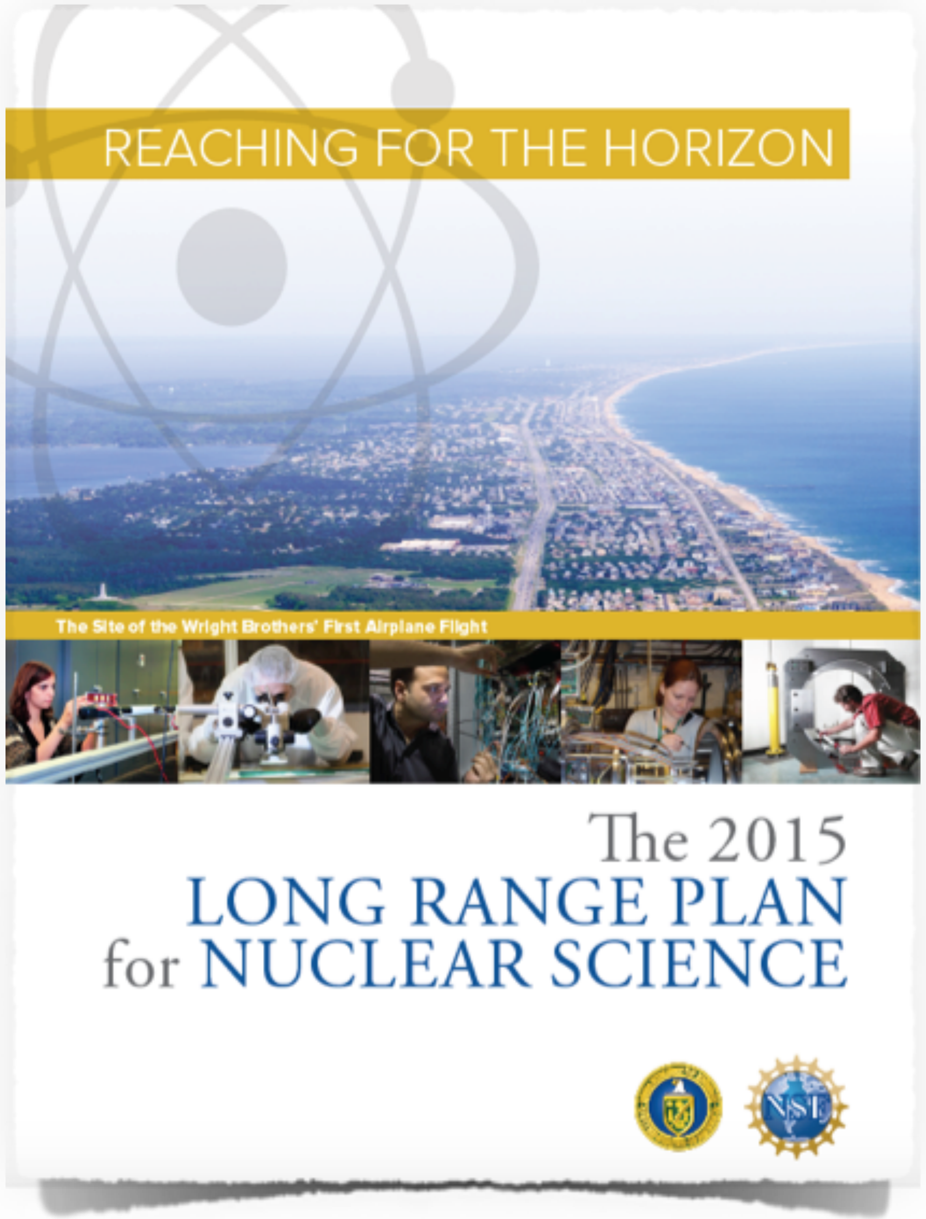
- Gauge generation (co-PI: Balint Joo)
  - Balint Joo - Sparse linear system solvers on emerging LCF-s (Cori, Summit, NERSC-9)
  - Boram Yoon - Sympletic PDE Integrators
  - Kate Clark (NVIDIA) - comms reduced solvers, Integrators
  - Kostas Orginos - 1 flavor methods
  - Xu Liu - Memory optimizations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

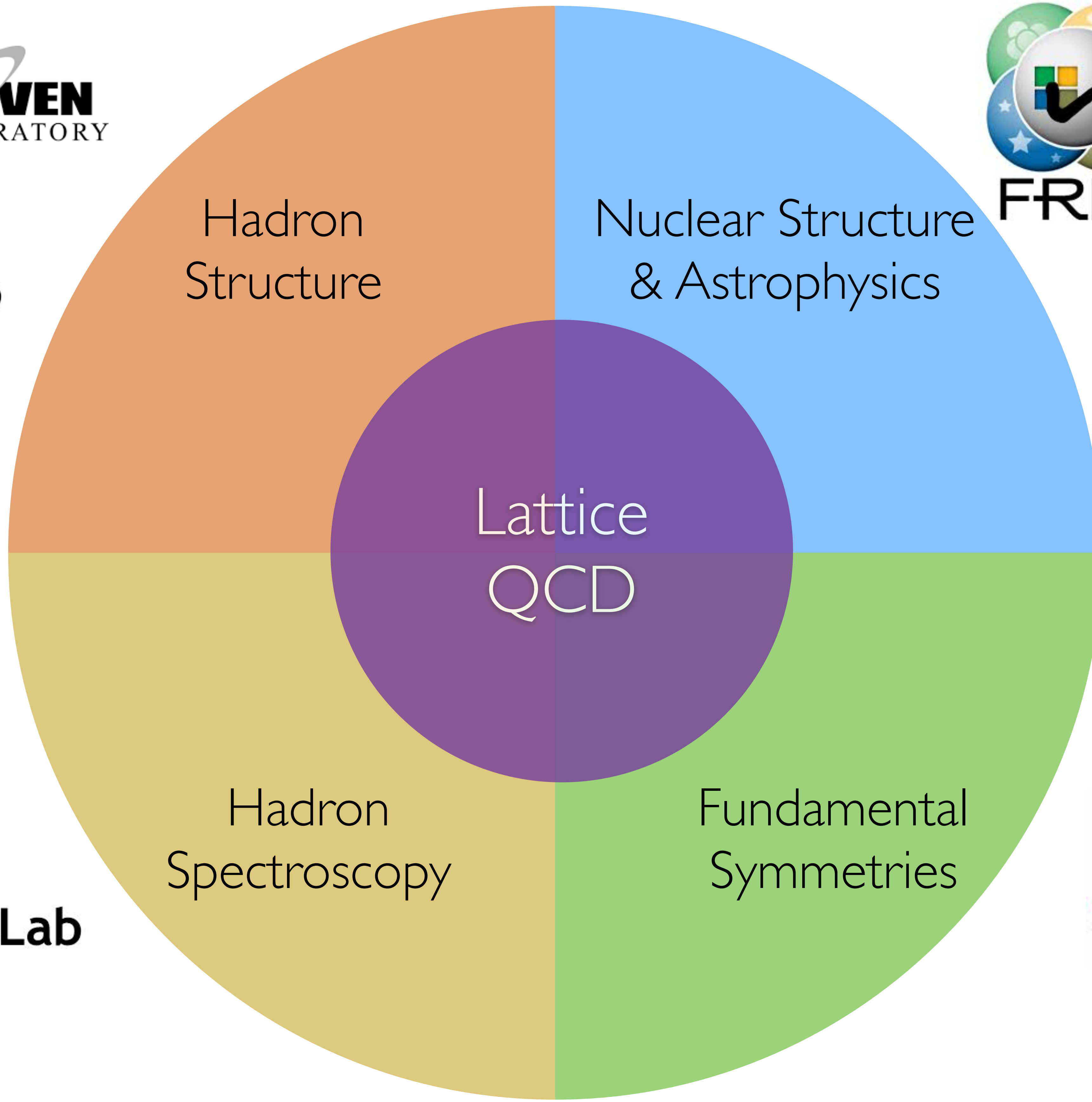
- Thermodynamics and Workflow (co-PI: Swagato Mukherjee)
  - Sergey Panitkin: PanDA/ATLAS workflow for LCF systems, multi-site campaigns, scheduling, file transfers & data integrity
  - Alexei Bazavov - transport coefficients

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



BROOKHAVEN NATIONAL LABORATORY

Jefferson Lab

FRIB

DUNE

Argonne NATIONAL LABORATORY

Los Alamos NATIONAL LABORATORY

SNS SPALLATION NEUTRON SOURCE

Jefferson Lab

Jefferson Lab

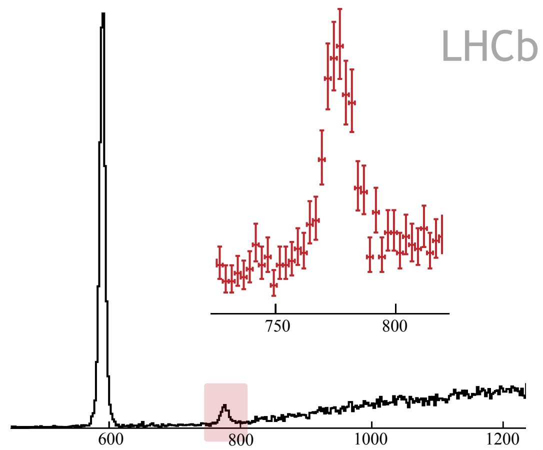
LQCD/NP Science & connection to Expt.

QCD, hadrons and the standard model

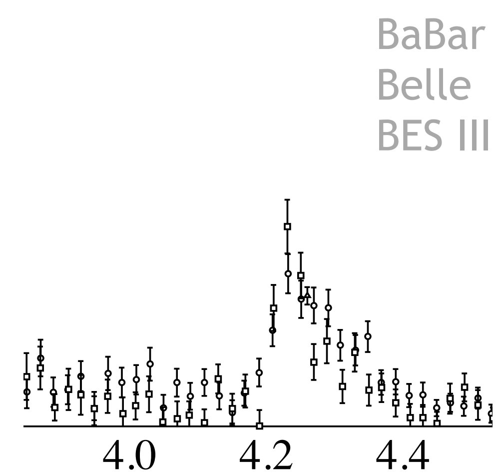
While **QCD** may be a solid part of the **standard model**, and **hadrons** are ubiquitous in HEP experiments, there remain significant mysteries in how **hadrons** are built from **quarks** and **gluons**

unexpected ?

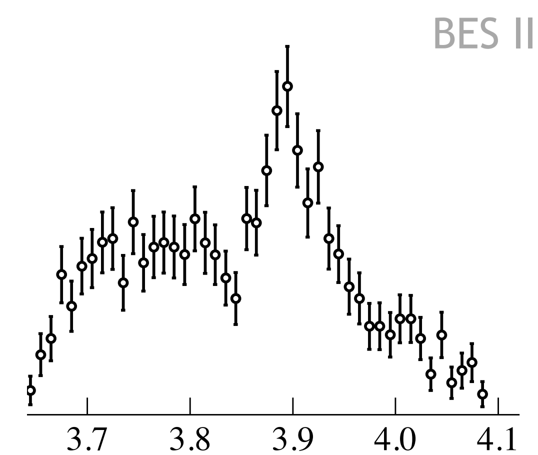
$X(3872) \to \pi\pi J/\psi$



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



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



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

$f_0(500)$ or σ [g]
was $f_0(600)$

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

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

$f_0(980)$ [j]

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

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

$K_0^*(800)$
or κ

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

$a_0(980)$ [j]

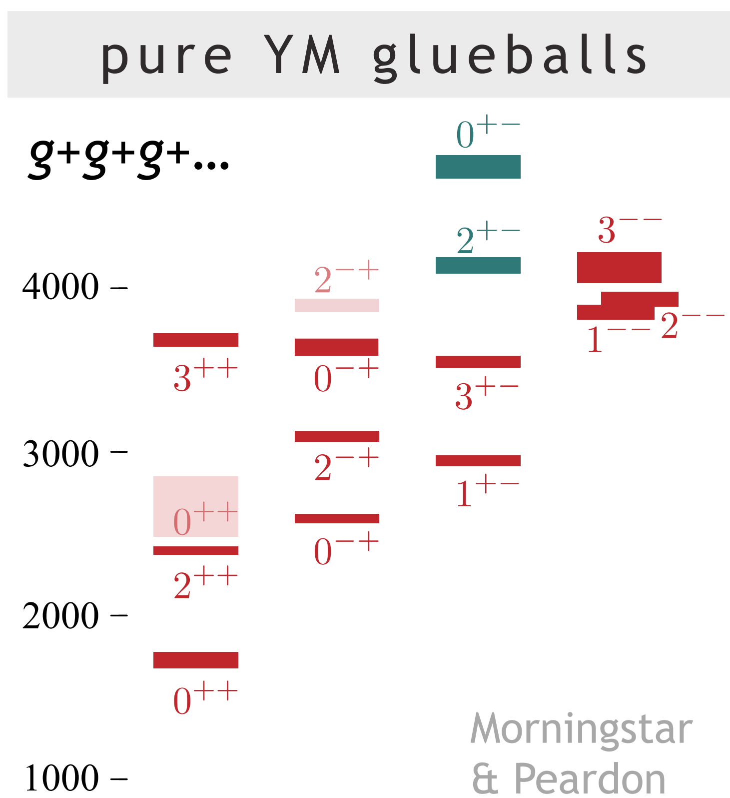
$I^G(J^{PC}) = 1^-(0^{++})$

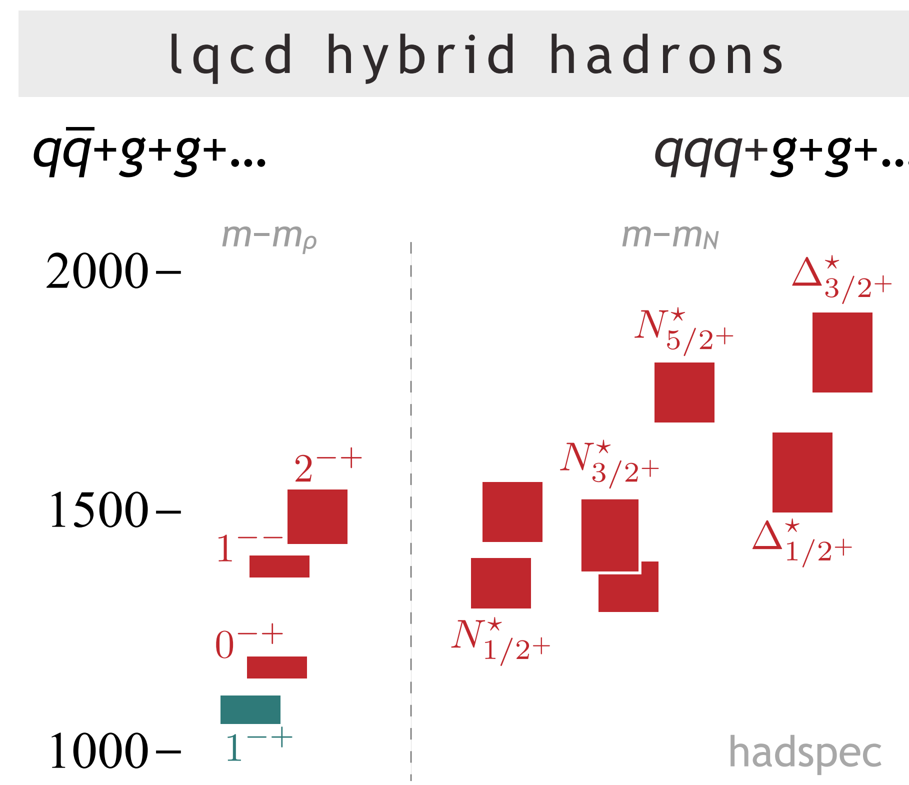
Mass $m = 980 \pm 20$ MeV
Full width $\Gamma = 50$ to 100 MeV

QCD, hadrons and the standard model

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**

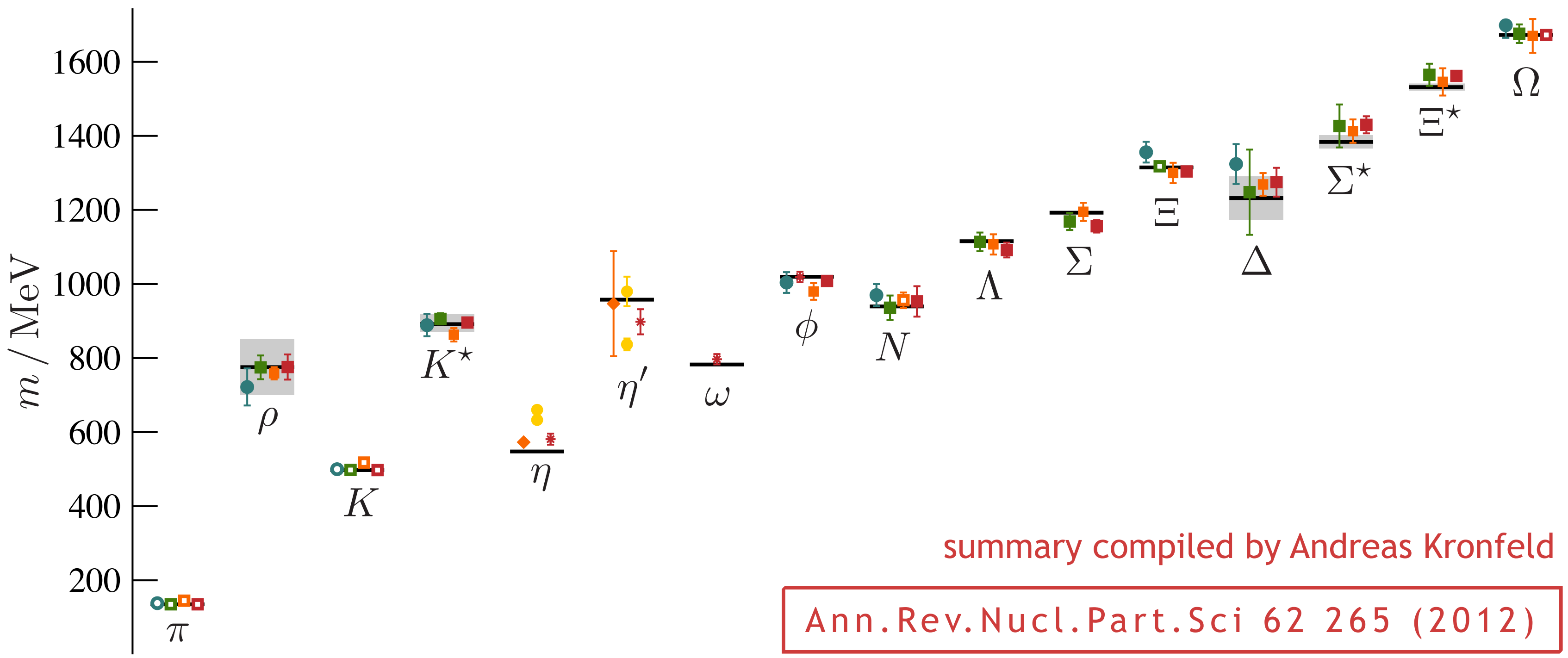
unobserved ?





Precise spectroscopy of stable hadrons

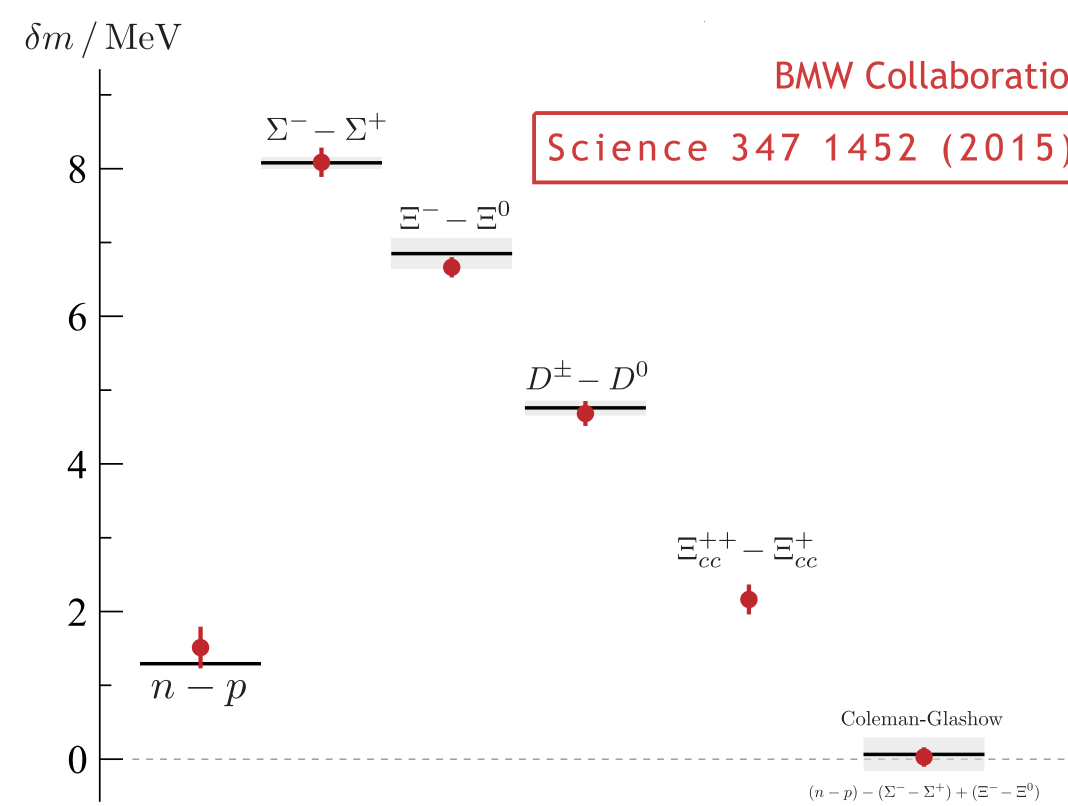
lattice qcd light hadron spectrum



summary compiled by Andreas Kronfeld

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

QCD+QED mass shifts



BMW Collaboration

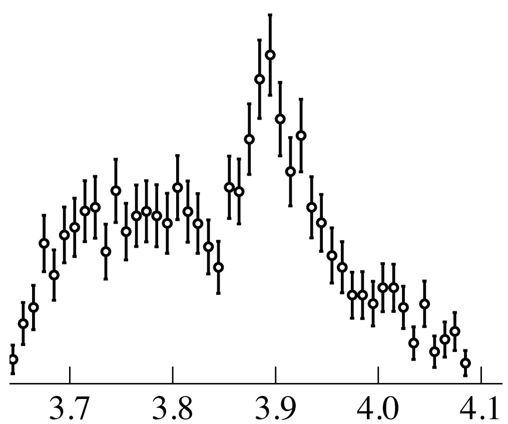
Science 347 1452 (2015)

Excited spectroscopy

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

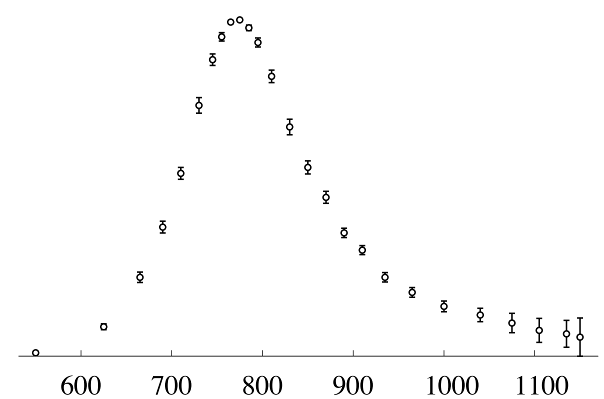
and they are **resonances** observed through their decays

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



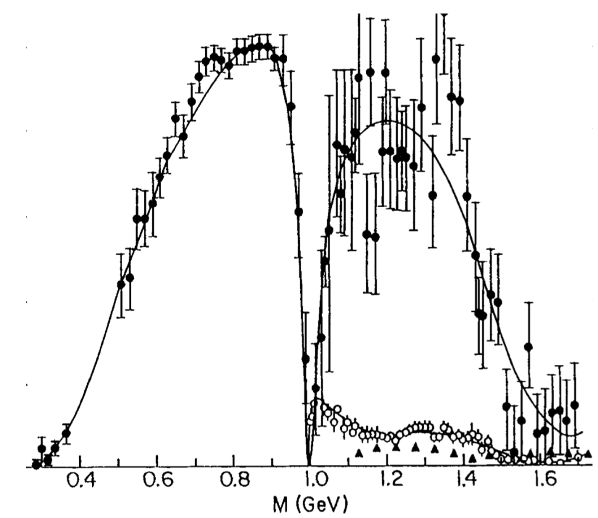
exotic

$\rho \to \pi\pi$



familiar

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



non-trivial

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

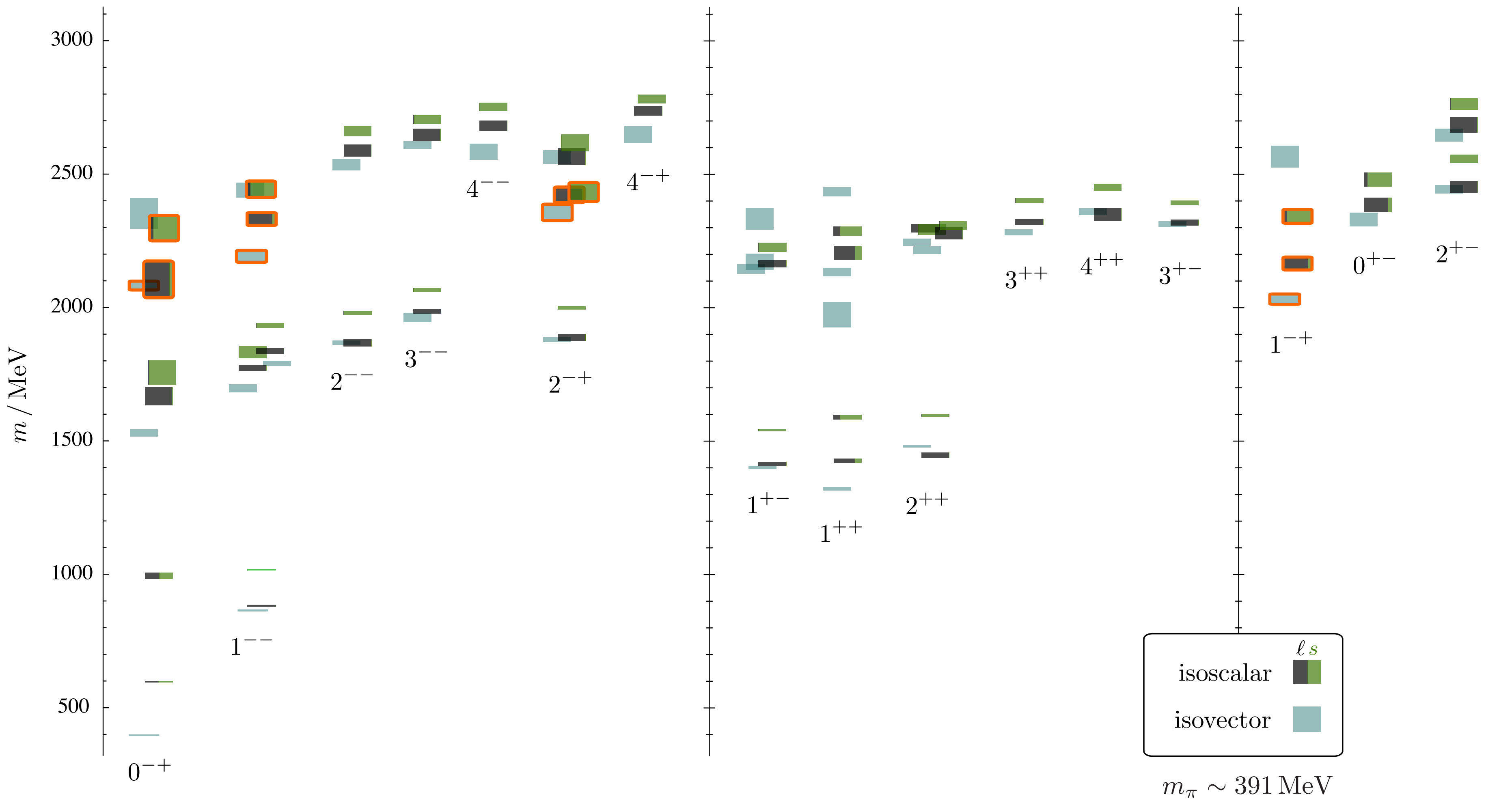
a faithful QCD calculation should give **all the scattering physics** at once ...

Lattice QCD & the excited hadron spectrum

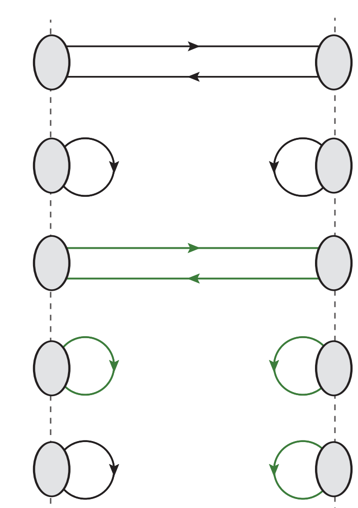
LQCD SciDAC project has pioneered novel techniques in lattice QCD

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

Exotics



'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

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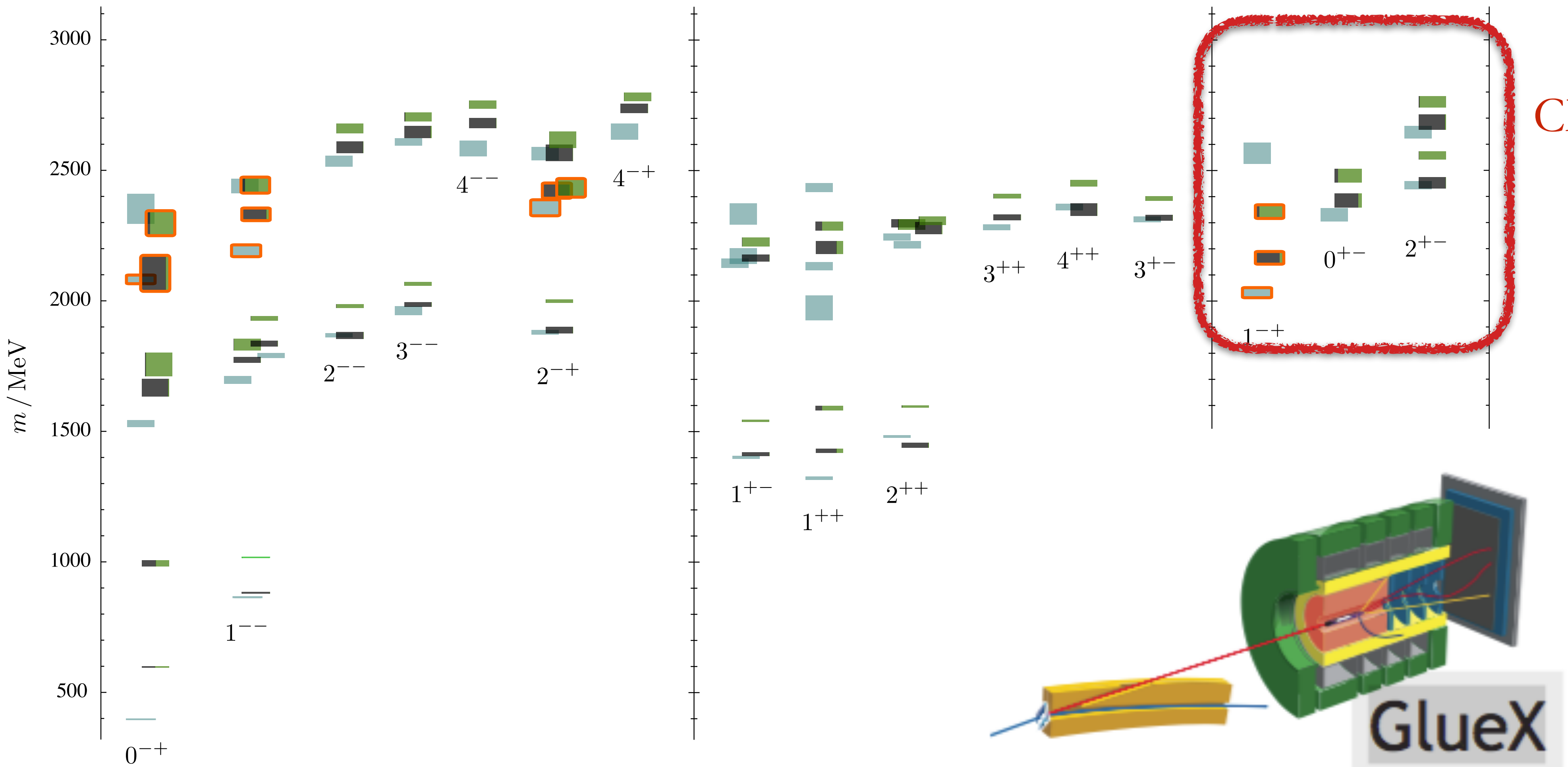
Hadron Spectroscopy - role of the glue

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

Exotics



Clear indication of exotics

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

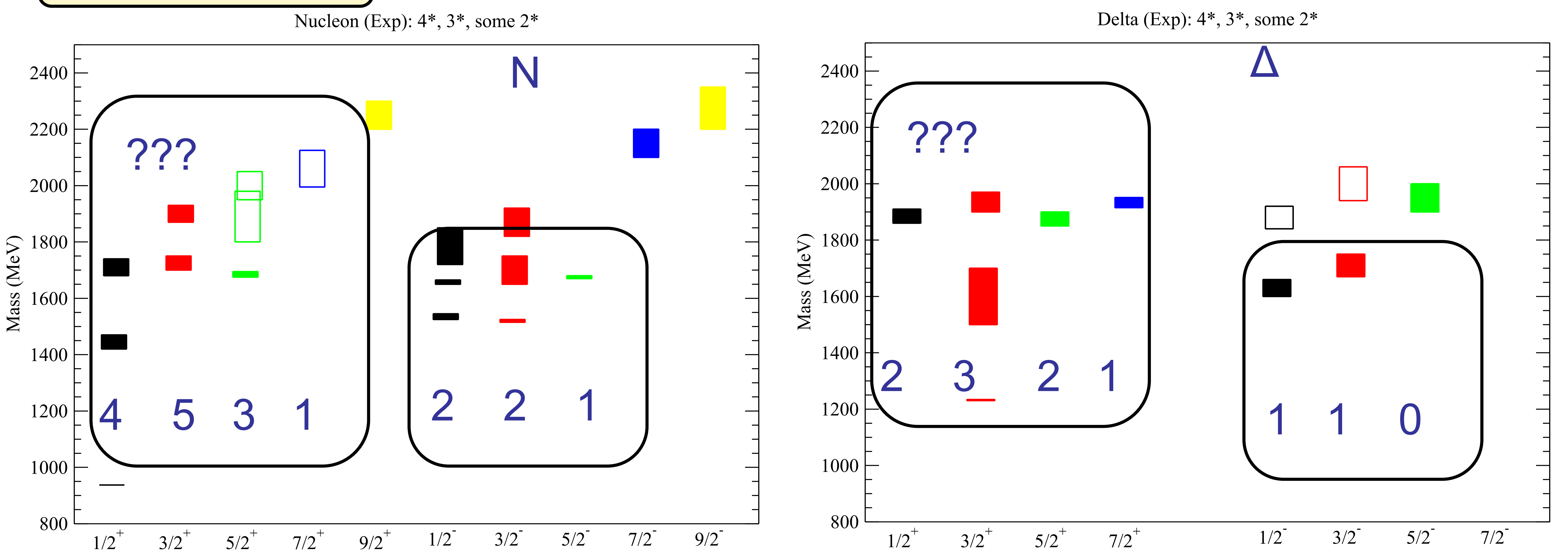
Where are the “Missing” Baryon Resonances?

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



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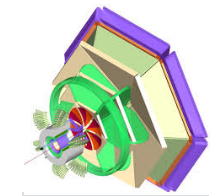
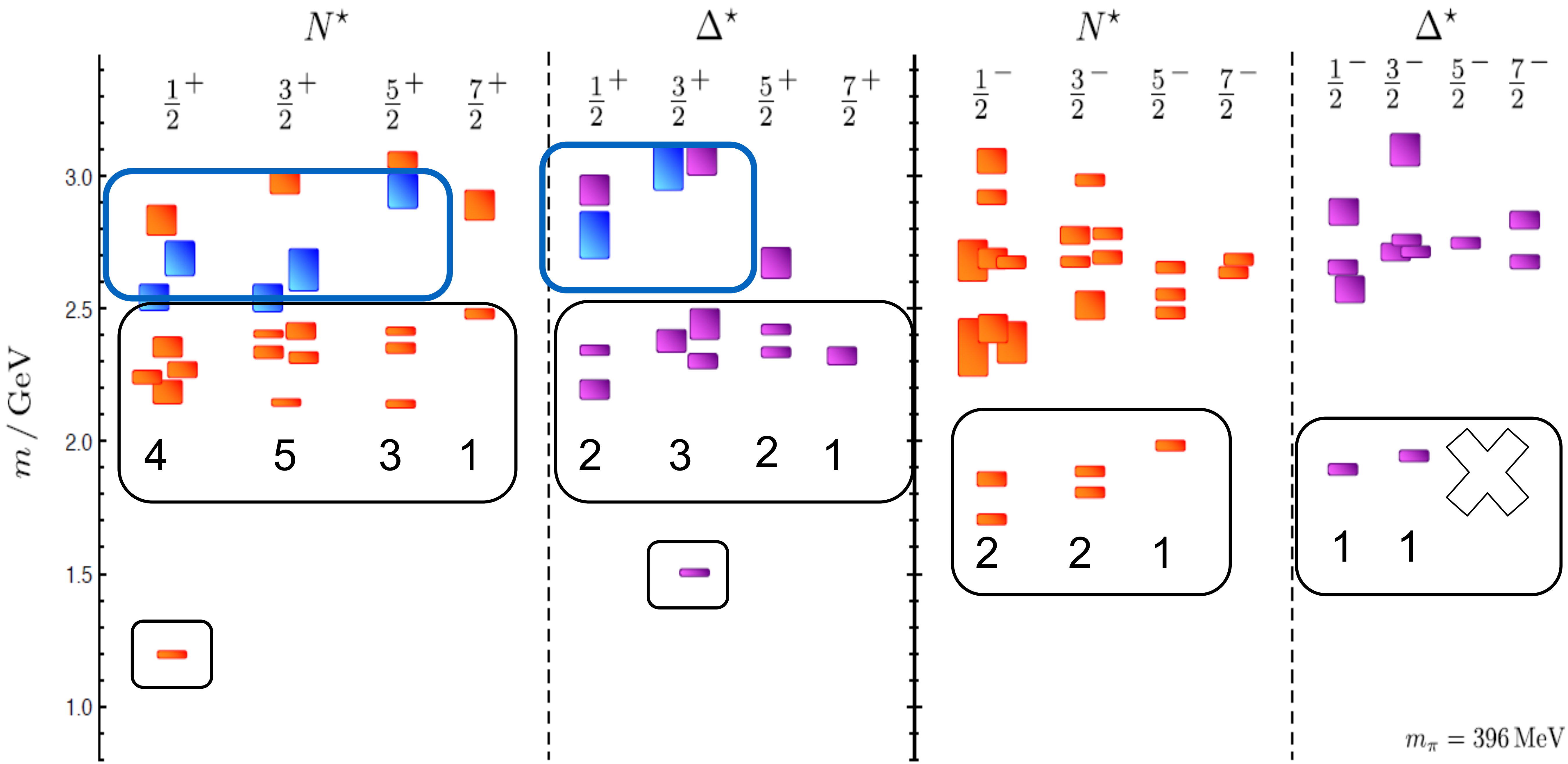
LQCD suggest no “missing" baryon states

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



Additional gluonic excitations within baryons

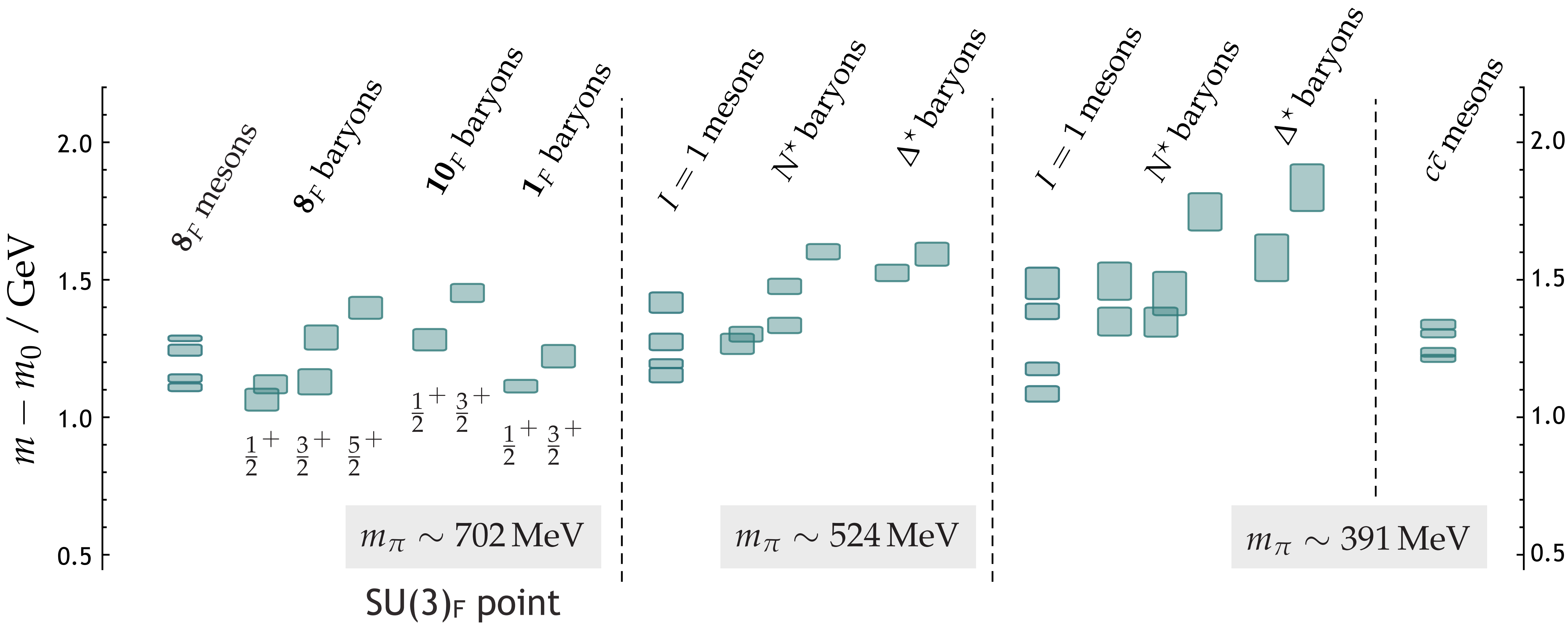
Spurred new expt. search in CLAS12@JLab



➡ Need observations in more decay channels

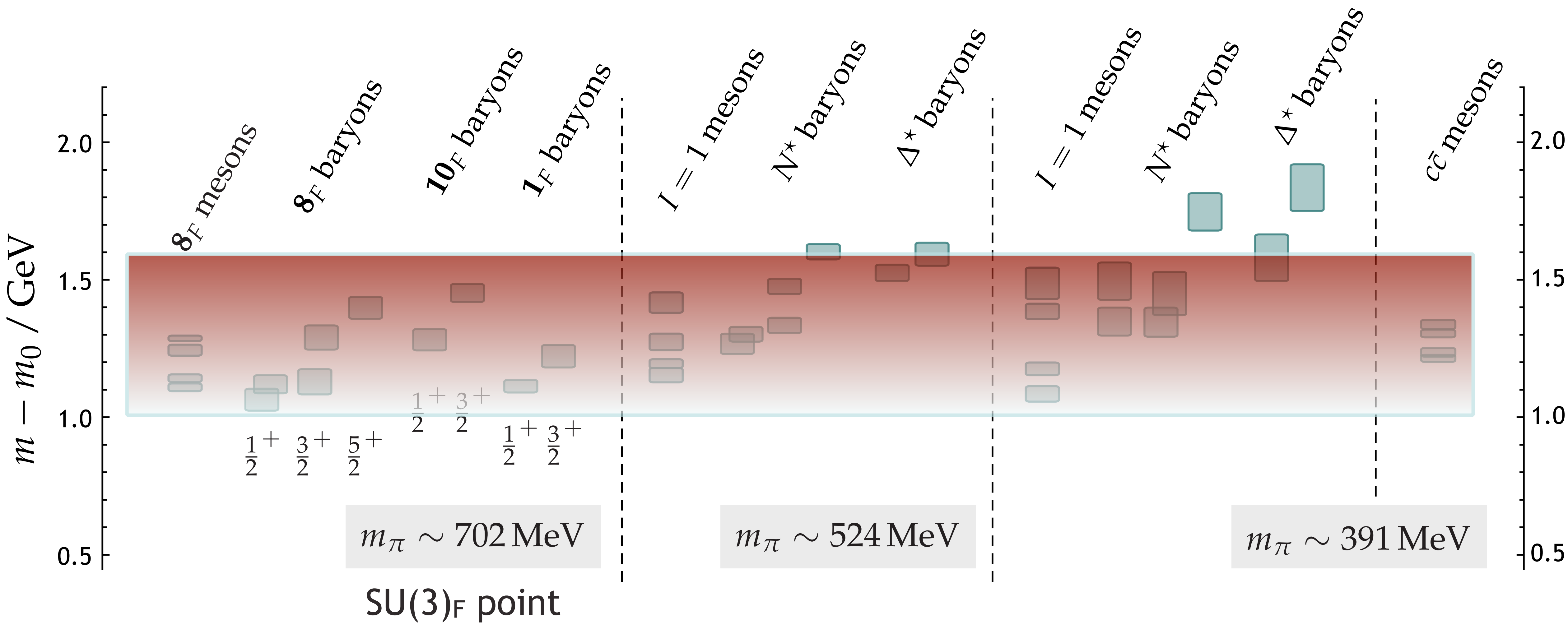
Hadron Spectroscopy - role of the glue

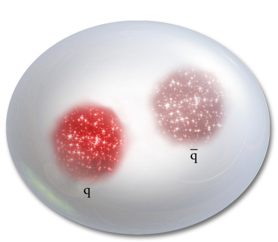
- Subtract the ‘quark mass’ contribution



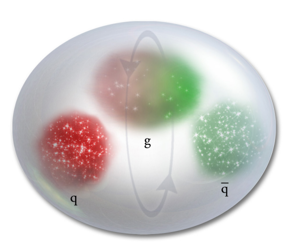
Hadron Spectroscopy - role of the glue

- Subtract the ‘quark mass’ contribution





Conventional Meson



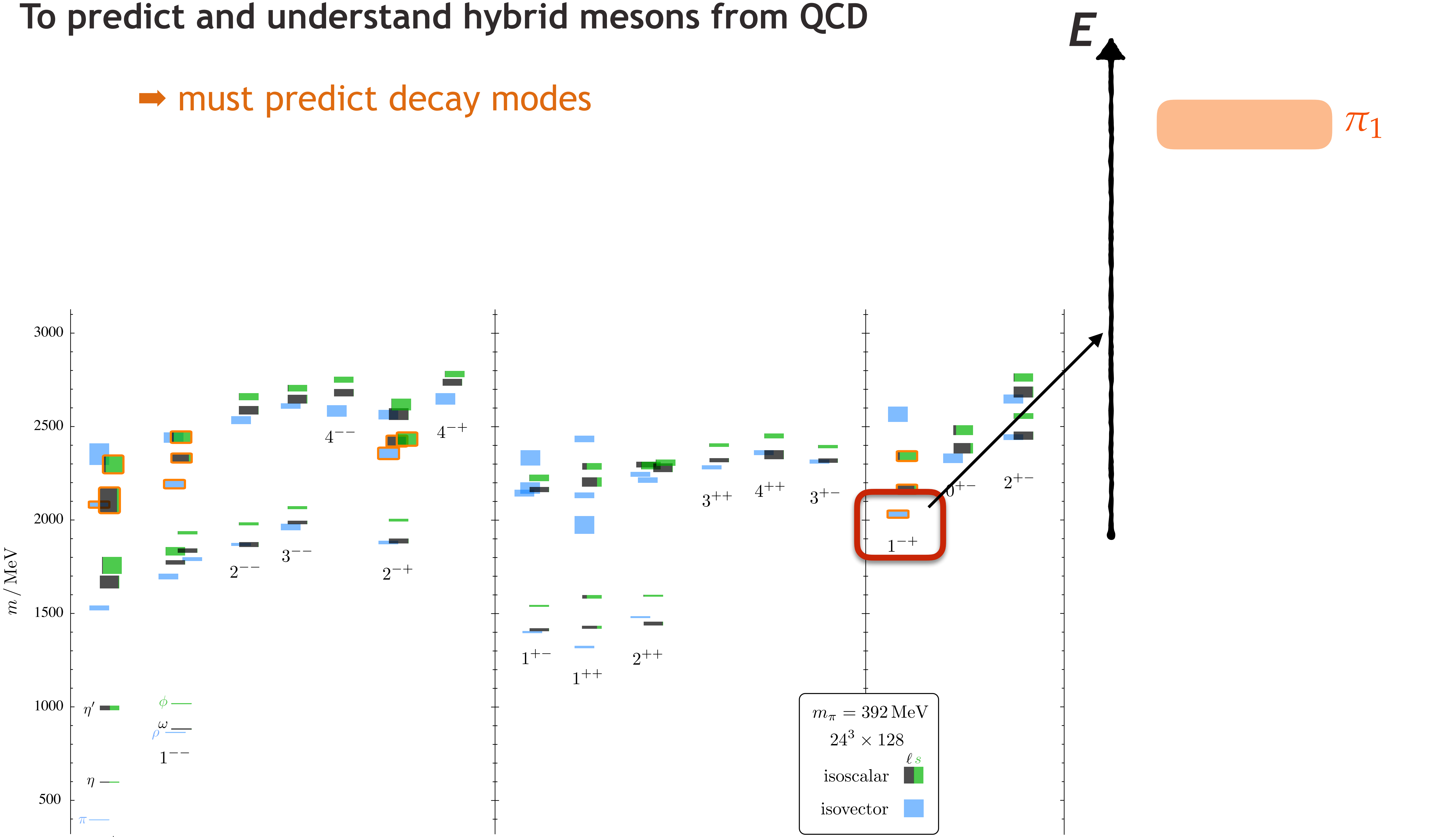
Hybrid Meson

Common energy scale of gluonic excitation ~ 1.3 GeV

Exotic hybrid mesons in QCD?

To predict and understand hybrid mesons from QCD

➡ must predict decay modes



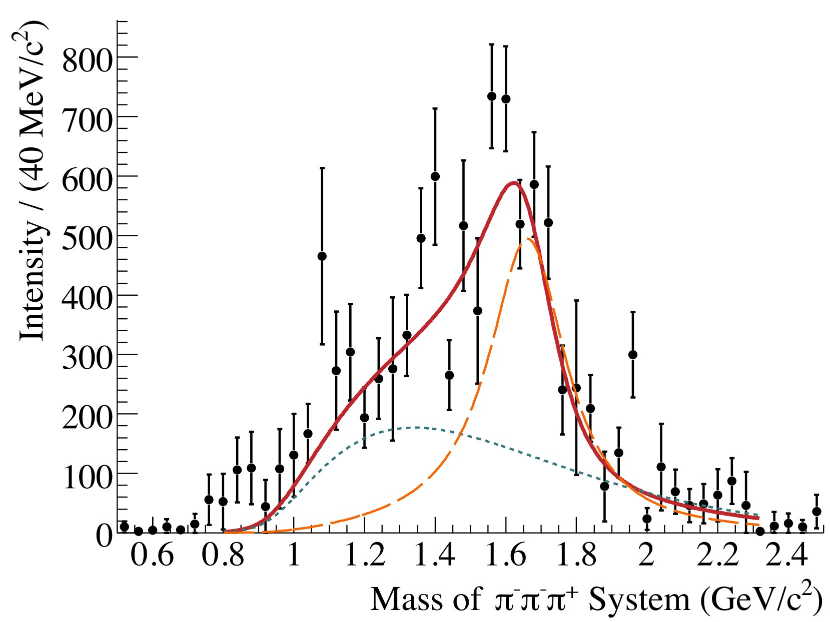
PRD83 111502 (2011)
PRD88 094595 (2013)

Exotic hybrid mesons in QCD?

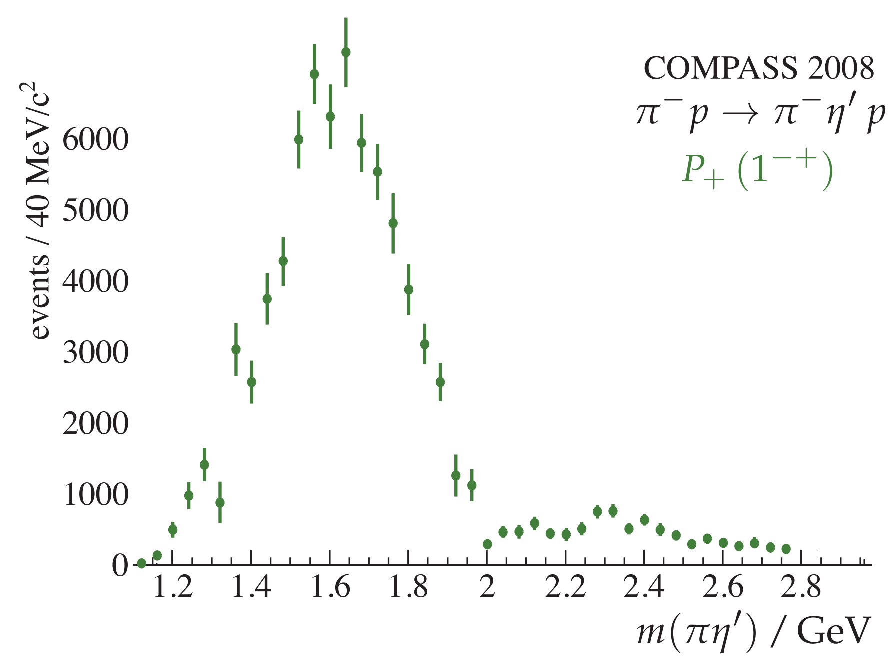
Excited states are resonances in scattering of lighter hadrons

We should see this in LQCD

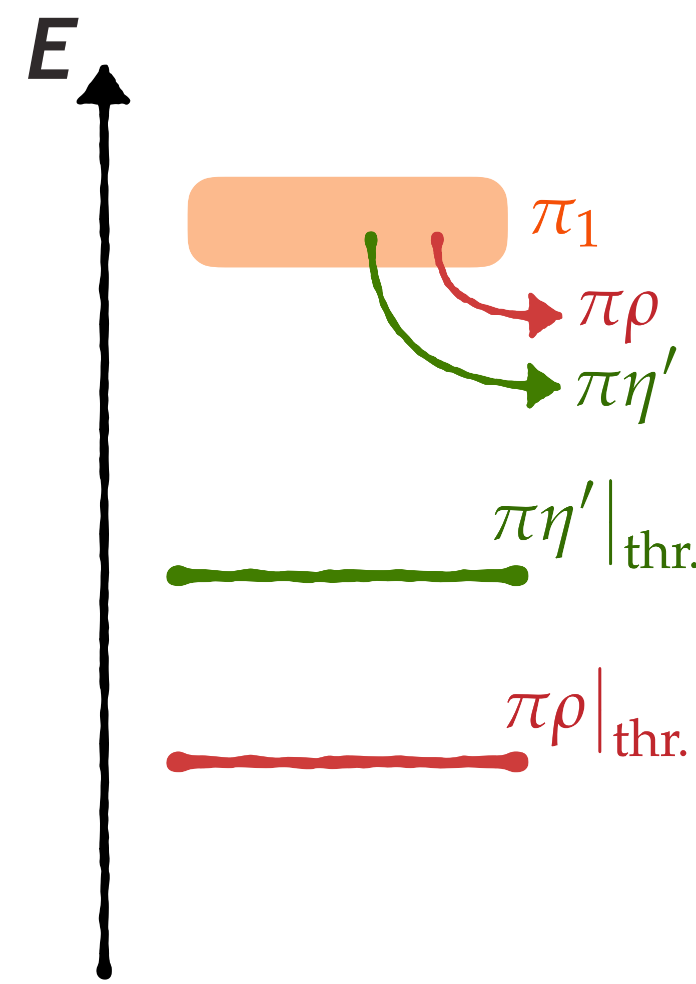
1^{-+} $[\rho\pi]_P$



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



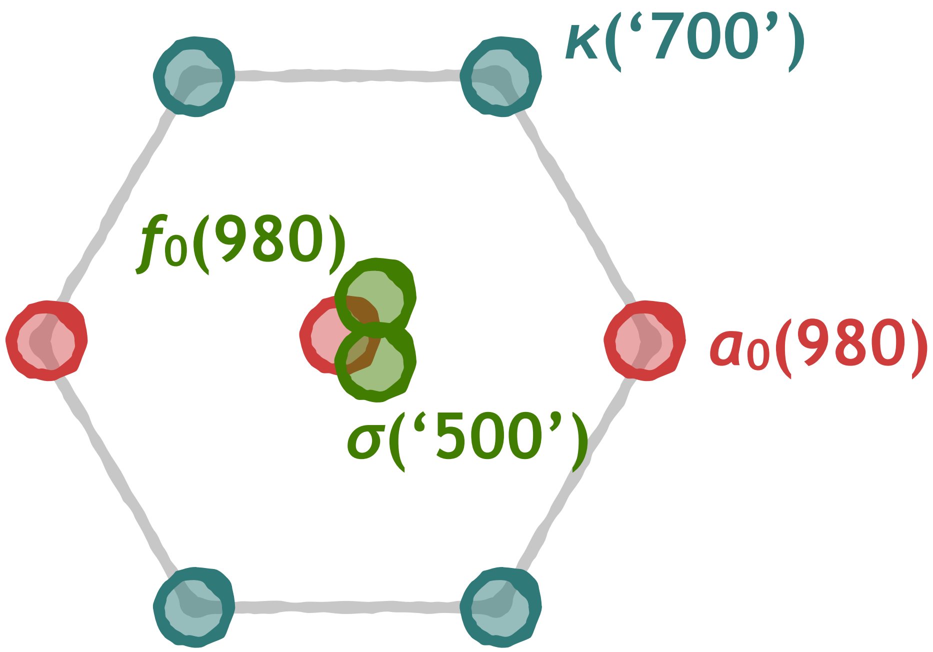
COMPASS Pb data
PRL104 241803 (2010)



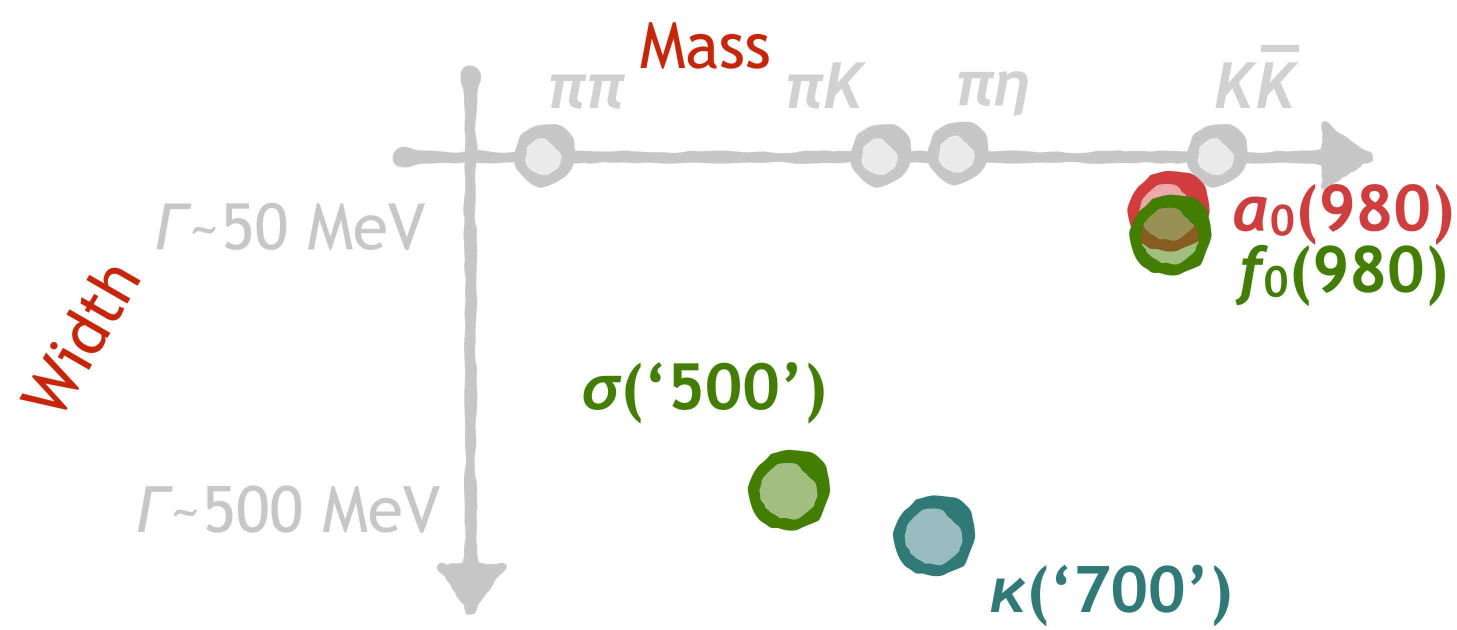
Hard - start with lower energies

Mysterious light scalar mesons

Conventional wisdom: an ‘inverted’ mass nonet



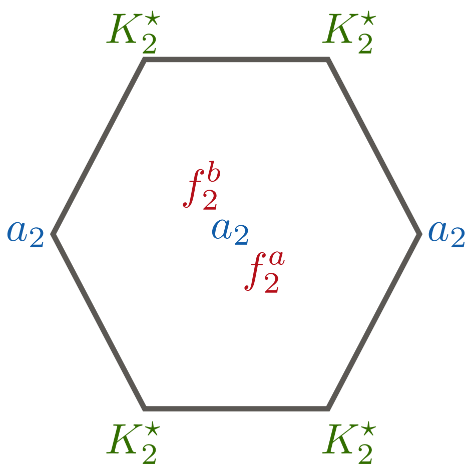
Similar? Vastly different masses & widths



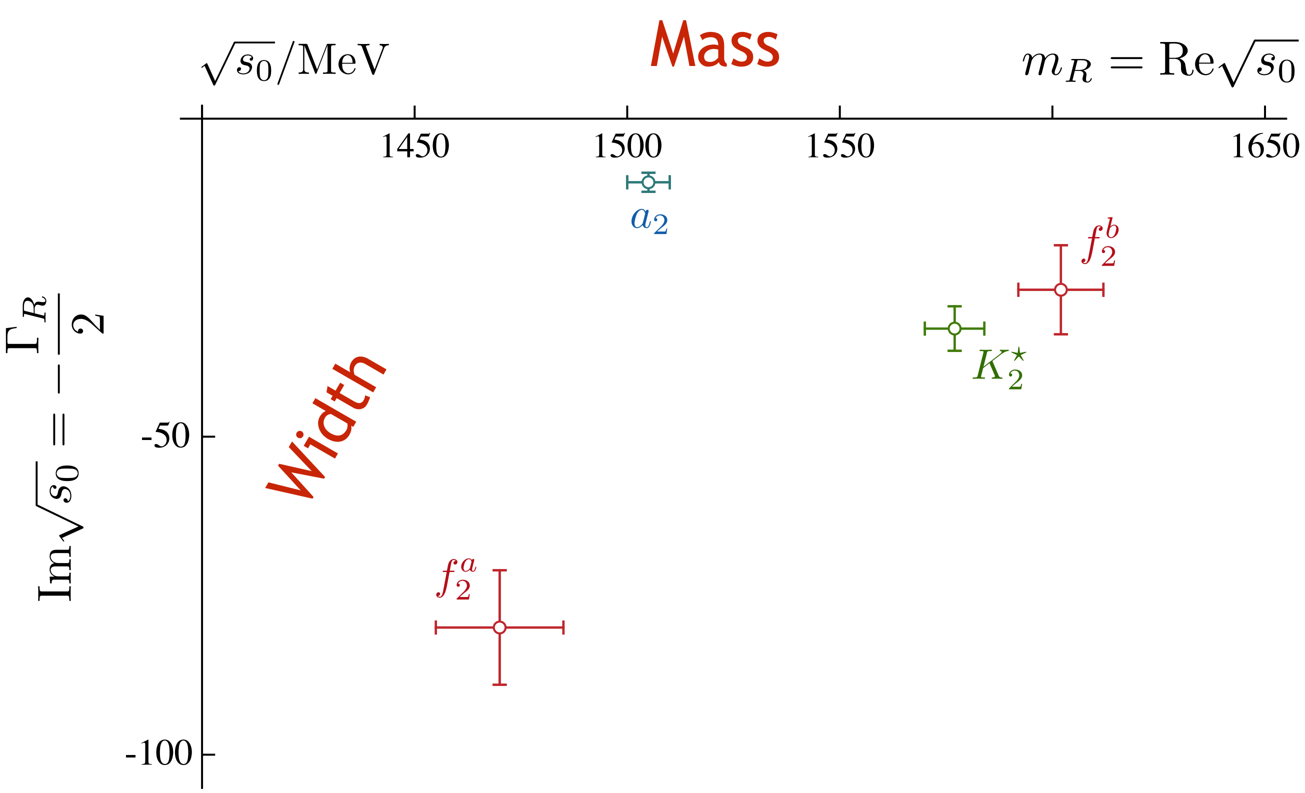
What does QCD have to say?

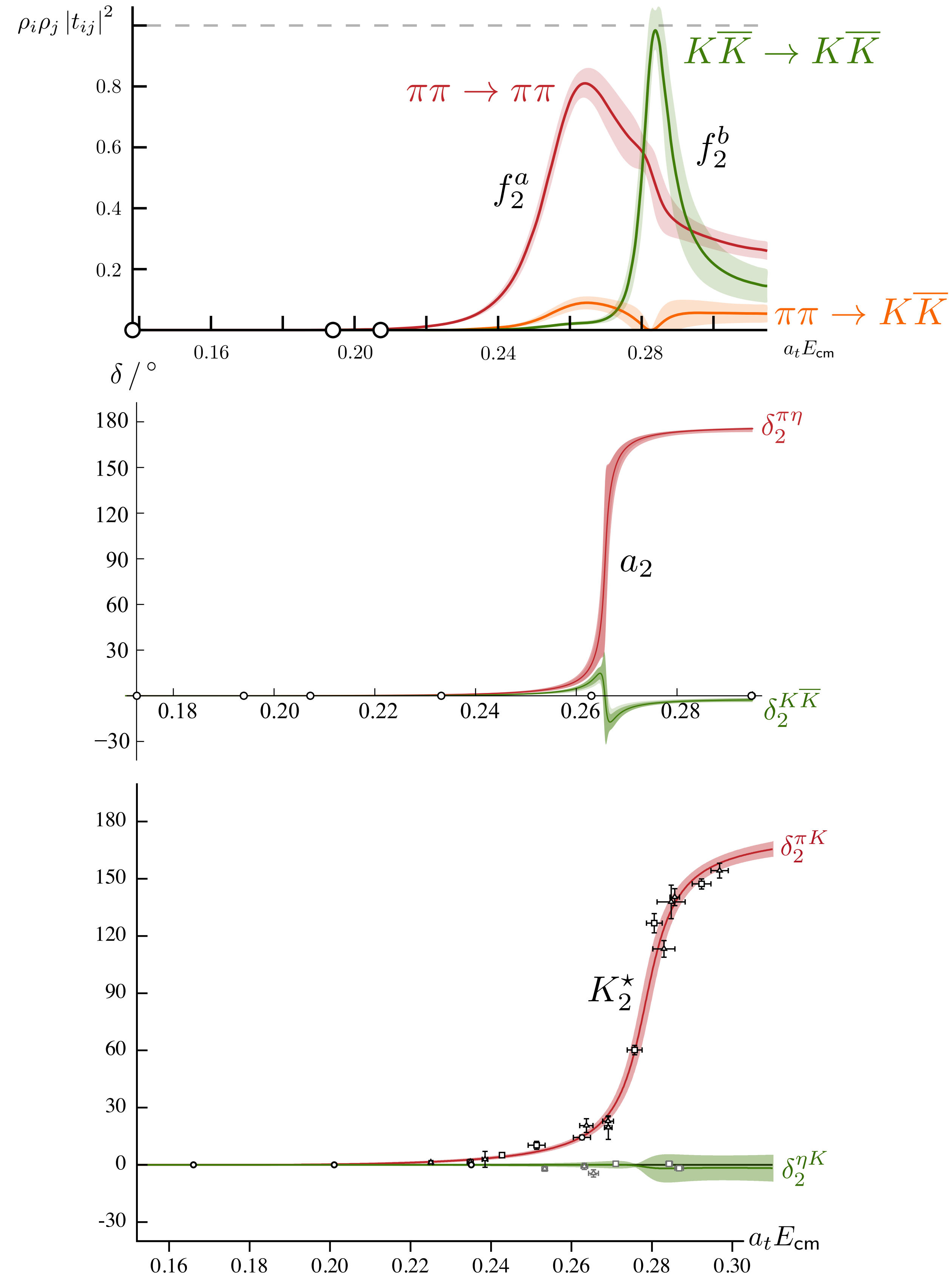
Lightest tensors at m_π=391 MeV

PRD97, 054513 (2018)

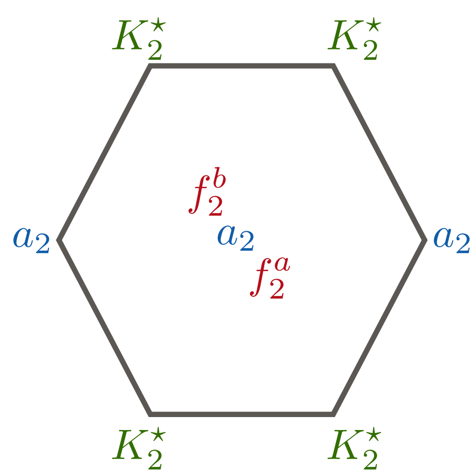


spin = 2

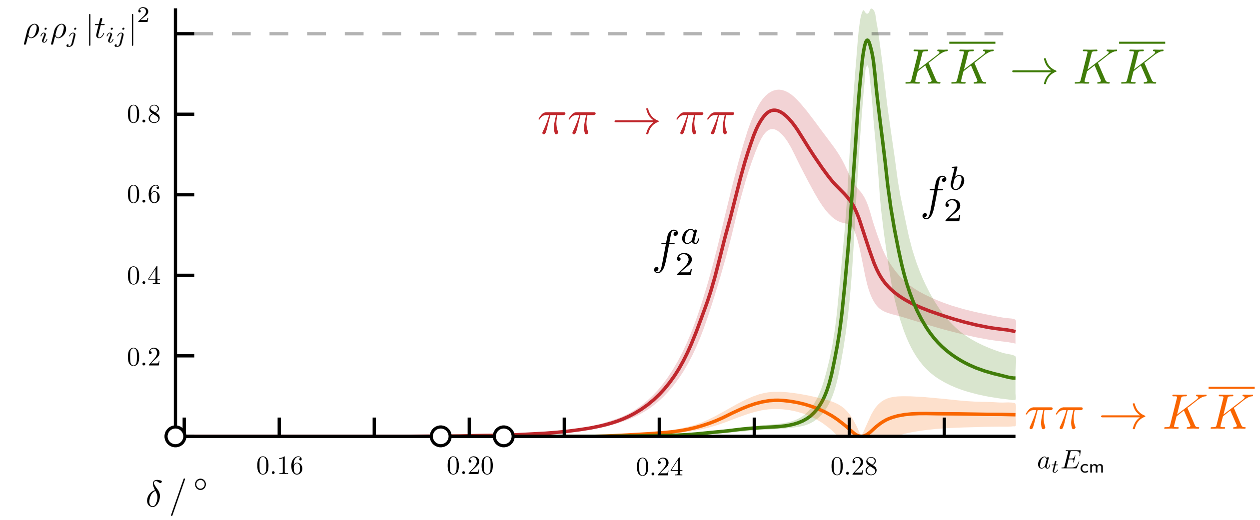




Lightest tensors at m_π=391 MeV

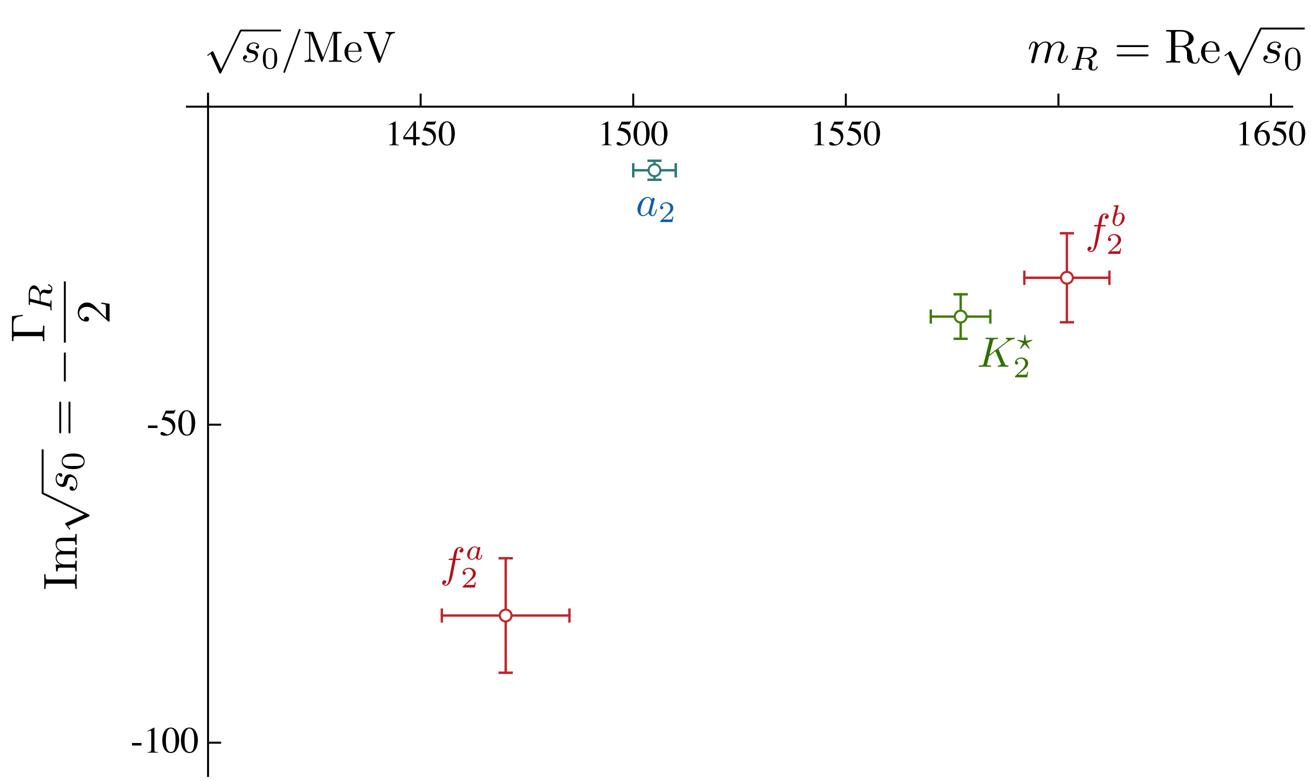


spin = 2



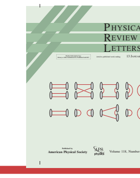
PDG $f_2(1270)$ → $\pi\pi$ 84% $f_2(1525)$ → $K\bar{K}$ 89%

flavor tagging by decays

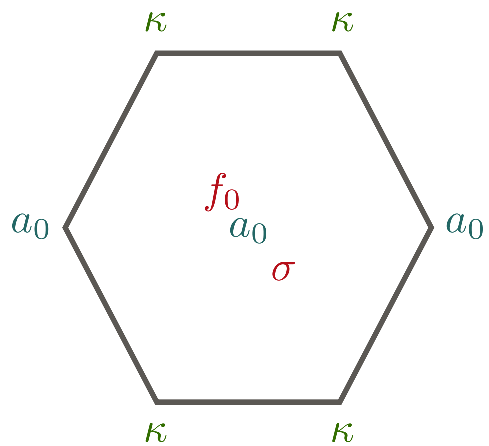


Used as motivation in
GlueX detector upgrade proposal

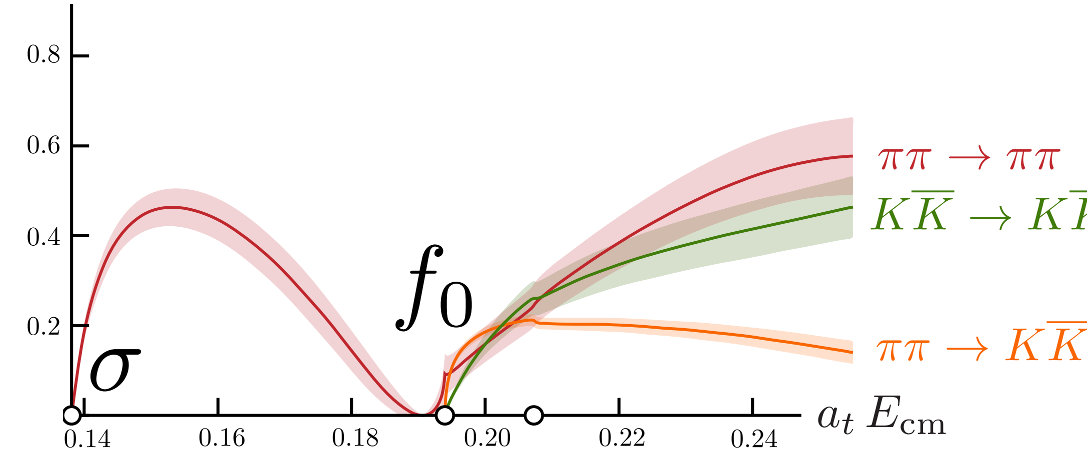
Lightest scalars at m_π=391 MeV

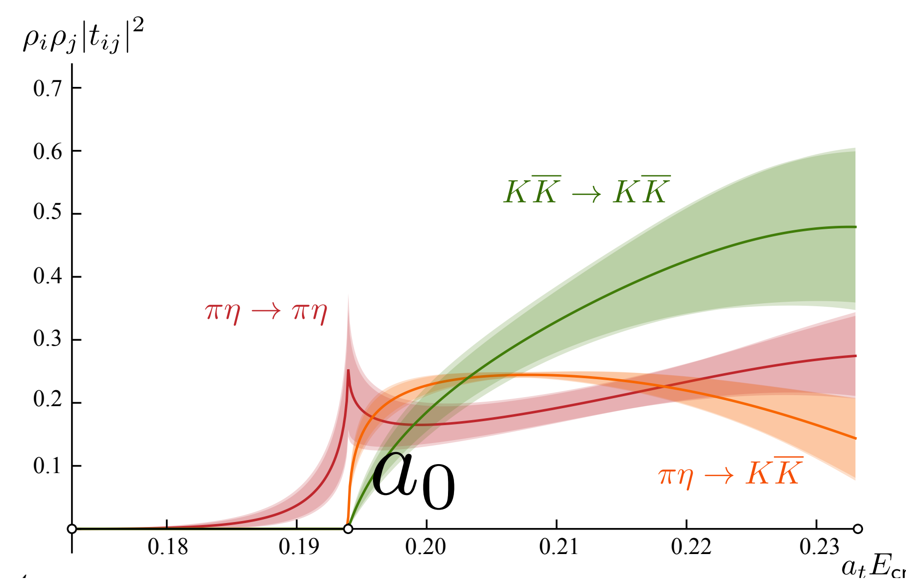


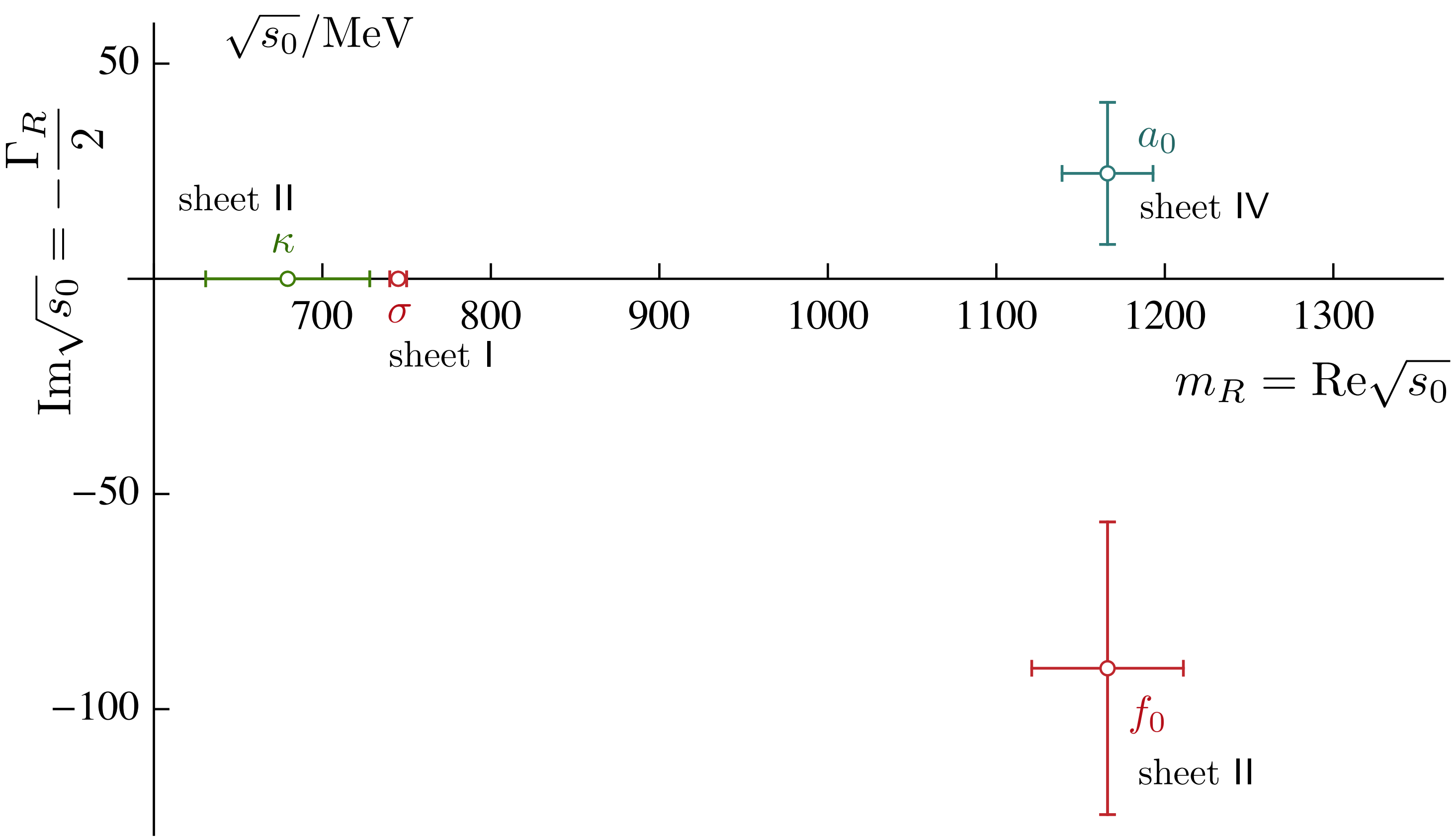
HadSpec: Phys.Rev.D97 (2018); Phys.Rev.Lett.118 (2017)

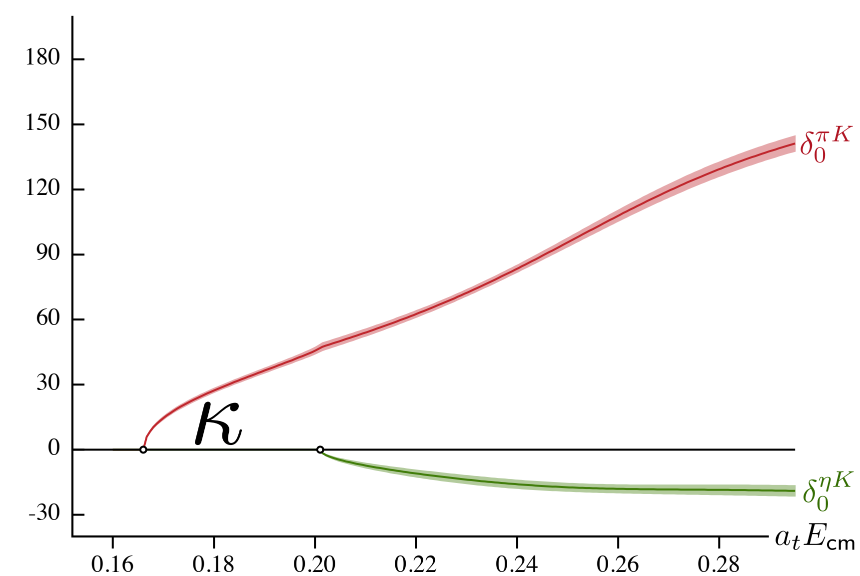


spin = 0

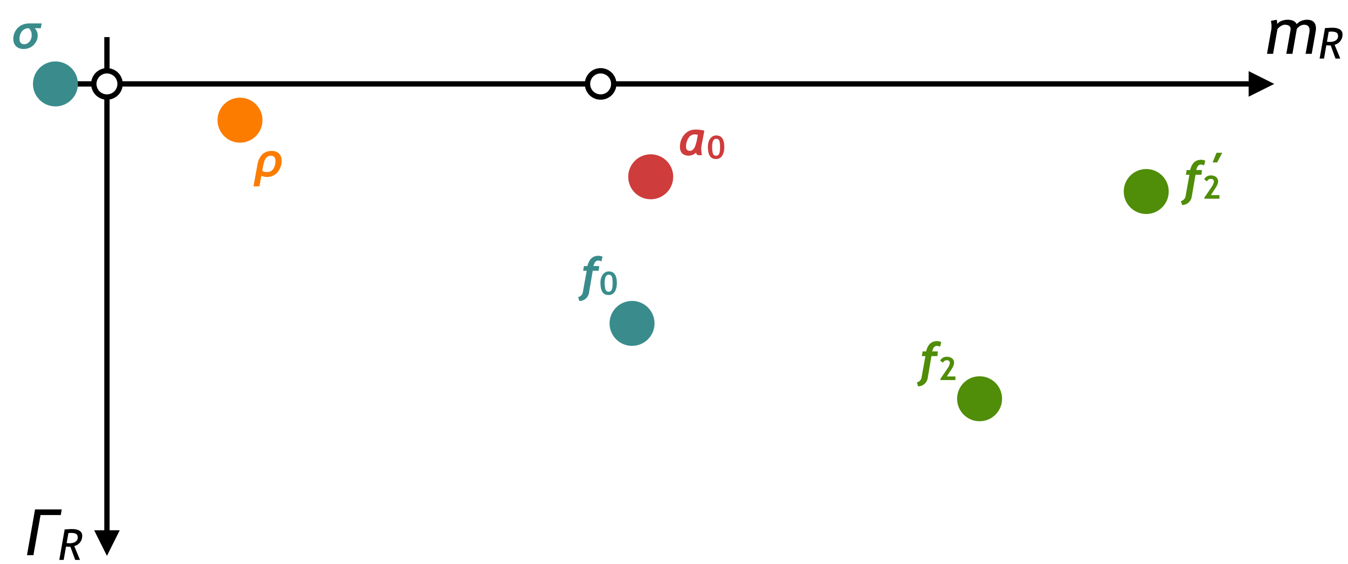








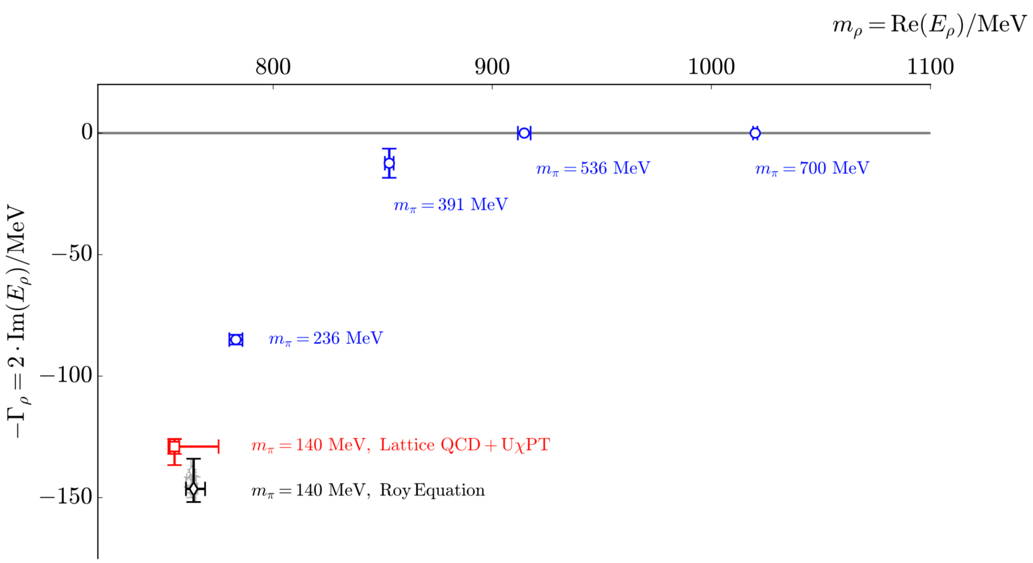
Light meson resonances at m_π~391 MeV

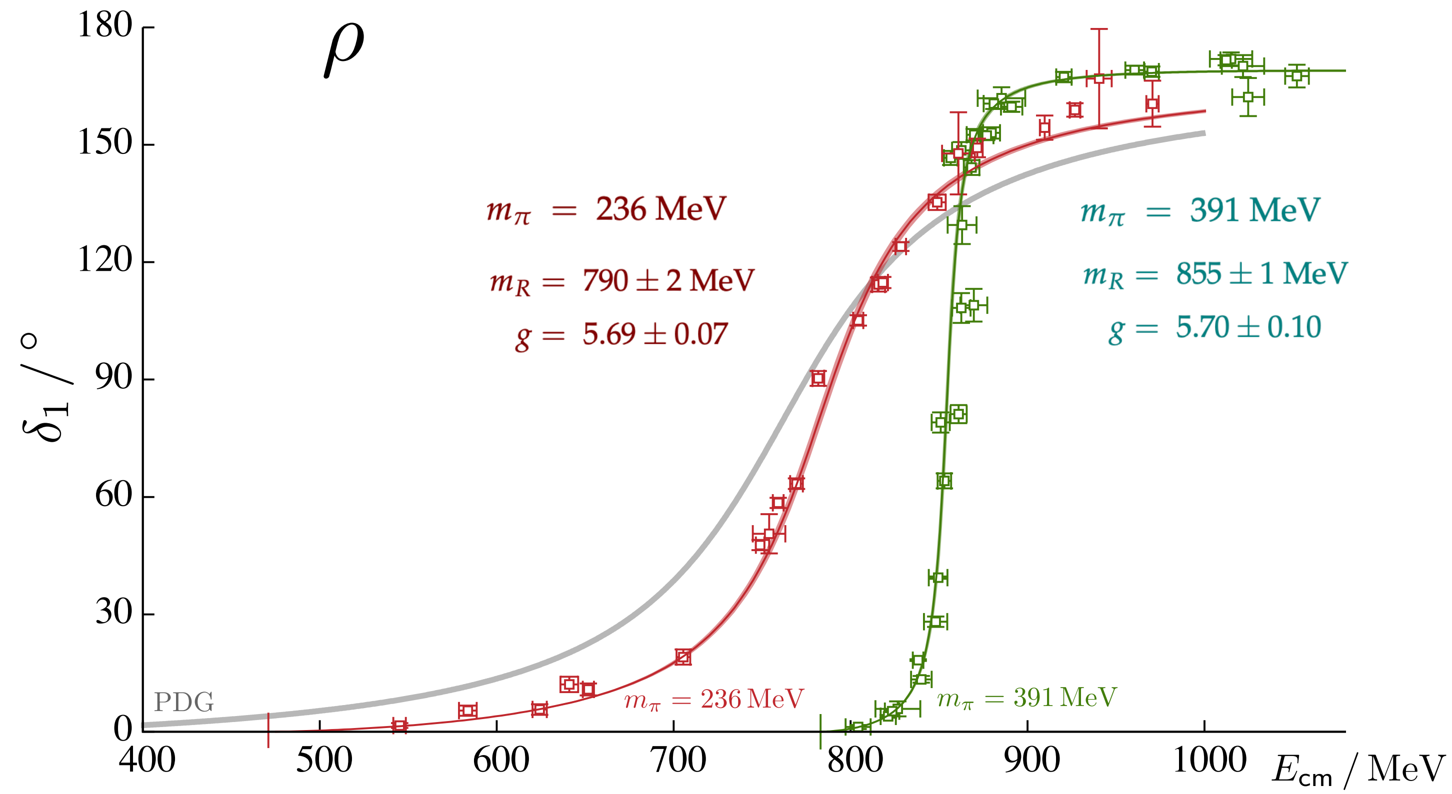


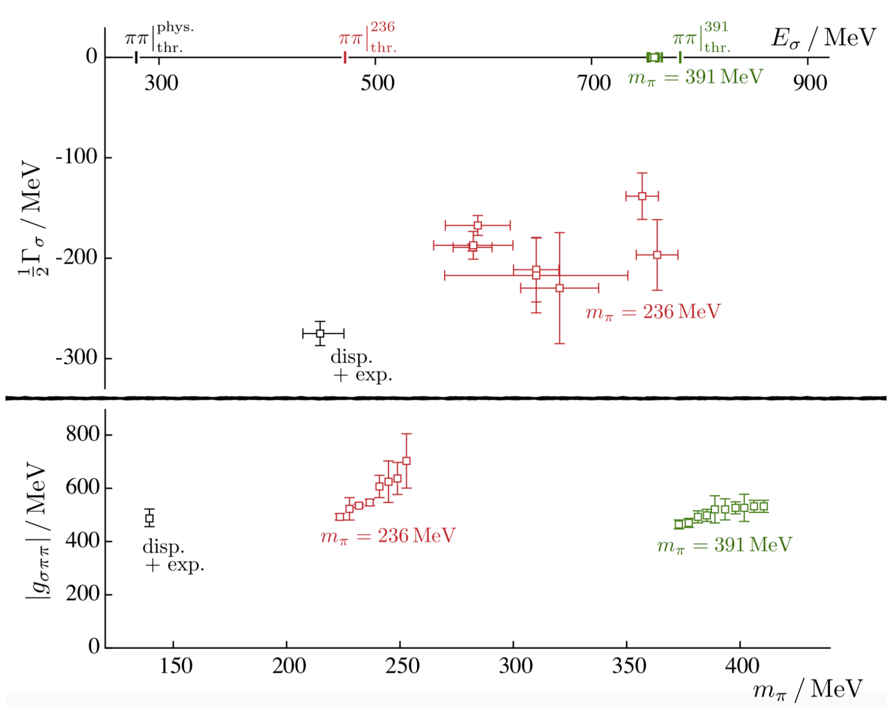
Have found the nonets of spin = 0, 1, 2 from QCD

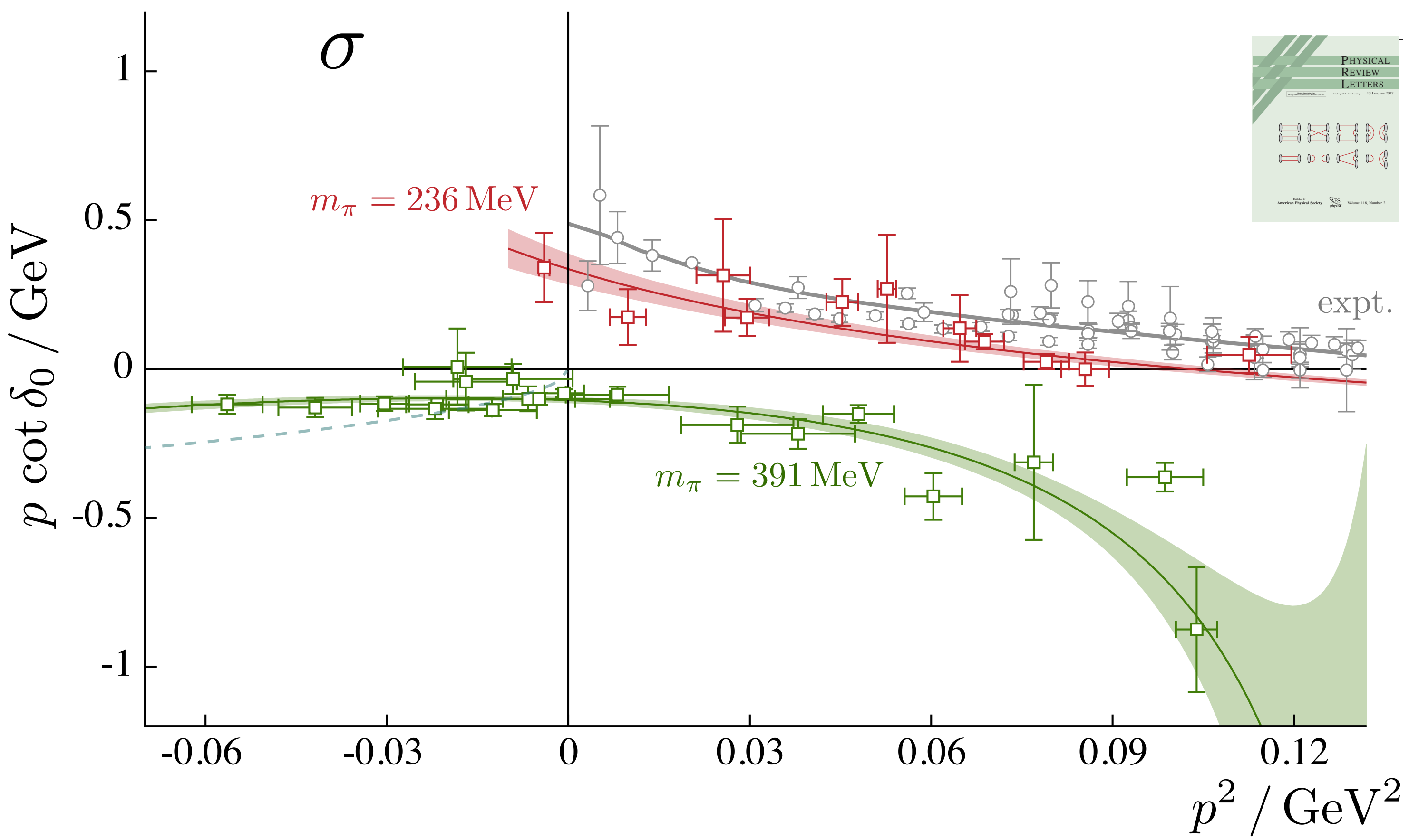
Thanks to SciDAC

Quark mass dependence: I=0 & 1









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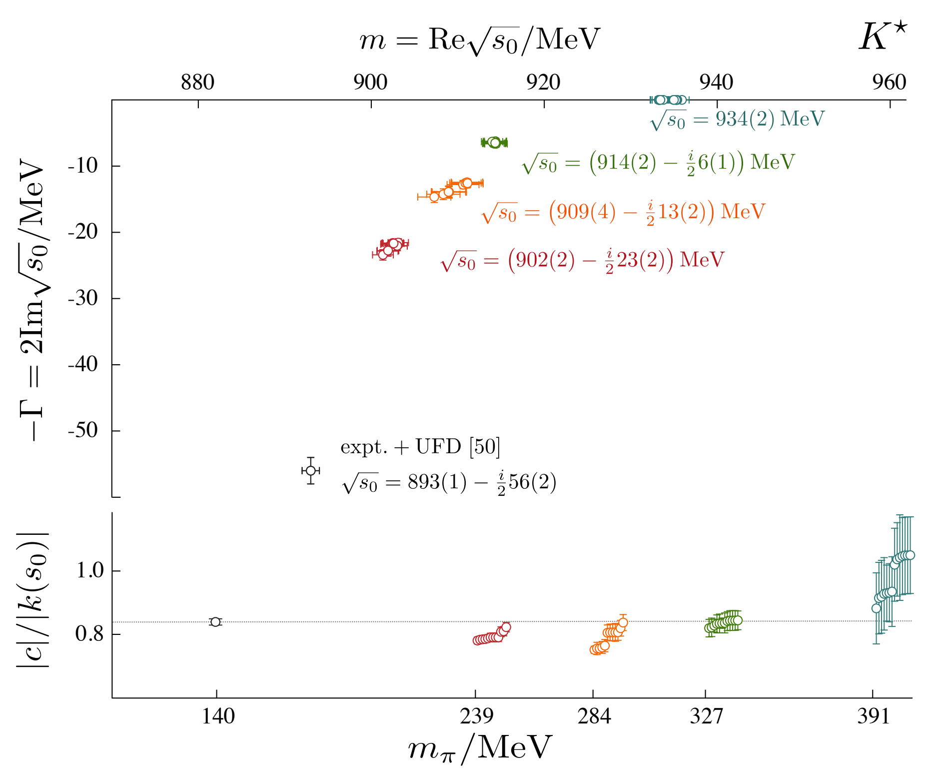
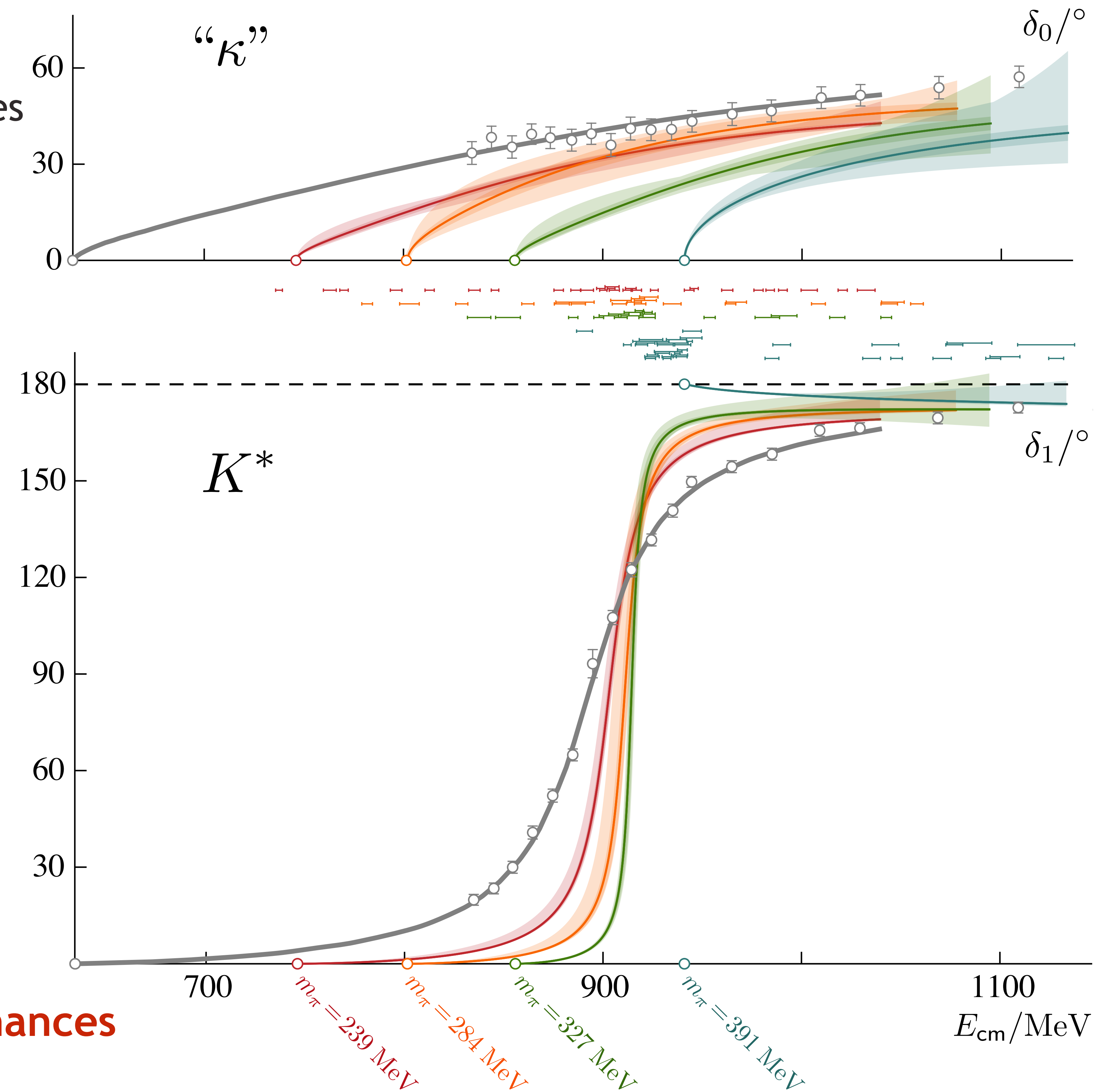
Quark mass dependence: I= 1/2

PRL in press

A more complicated story…
need “t” & “u”-channel amplitudes



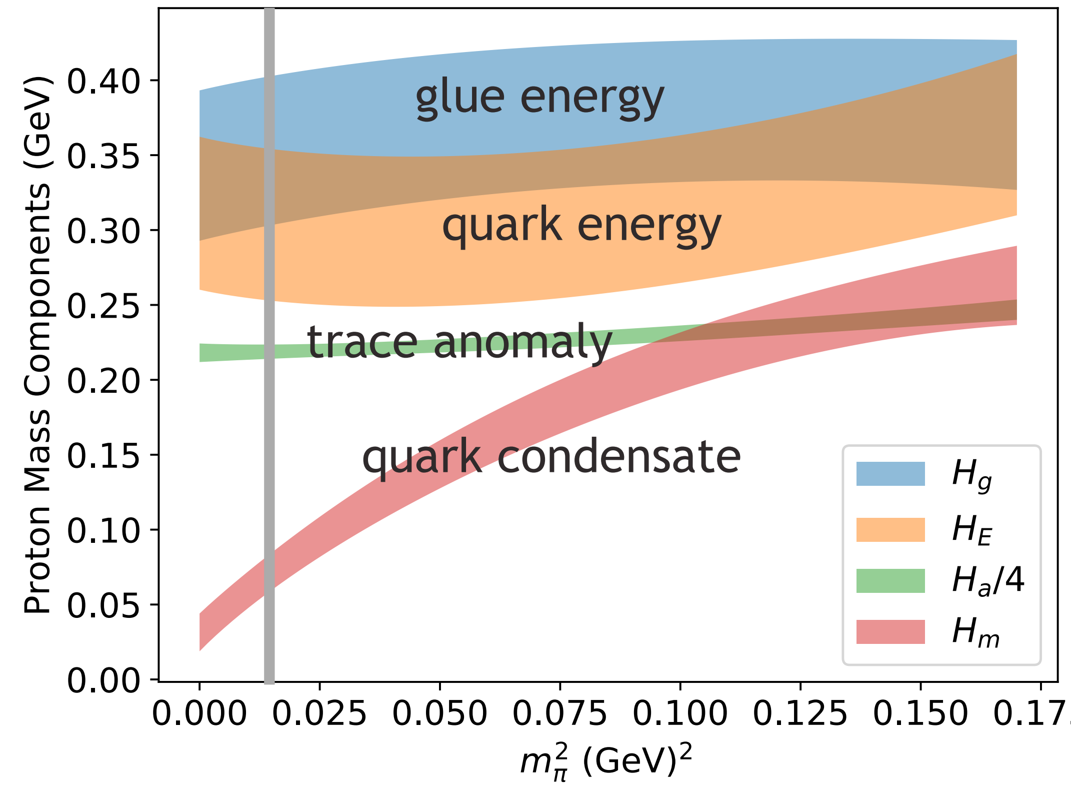


Message: LQCD can tackle resonances

Anatomy of the Proton Mass

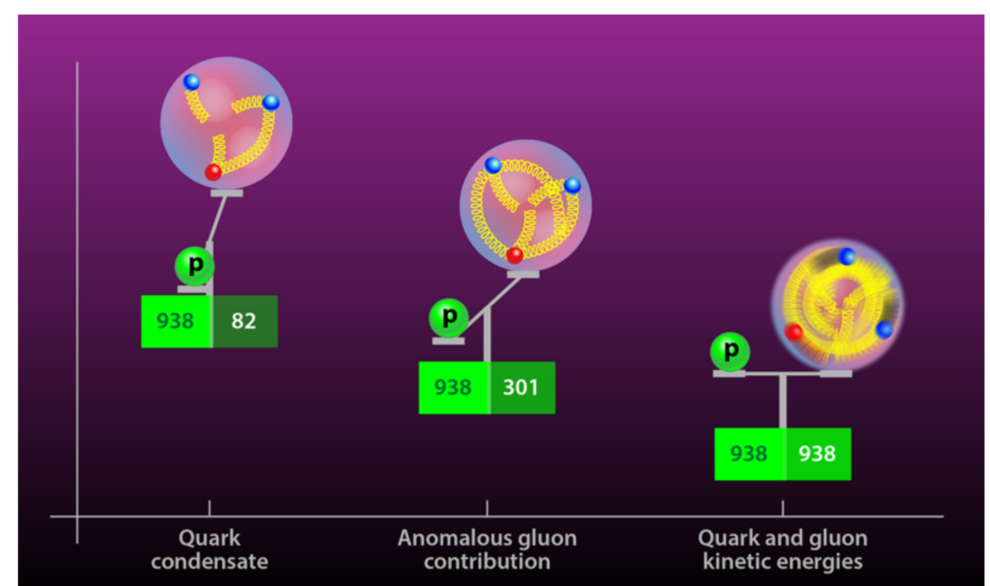
- Your mass comes from $M = E/c^2$ of the nucleons inside your atoms.

- The energy comes from:
  - quark masses (Higgs-Yukawa);
  - dimensional transmutation;
  - quark and gluon kinetic energies.



- Yang *et al*. (χQCD), Phys.Rev.Lett 121 (2018).

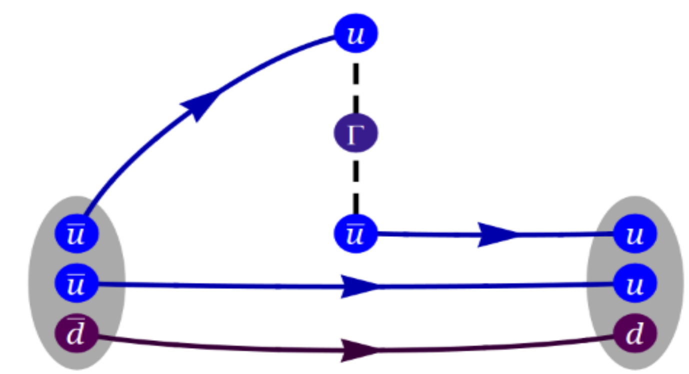
- ScienceNews! APS Physics! ☛

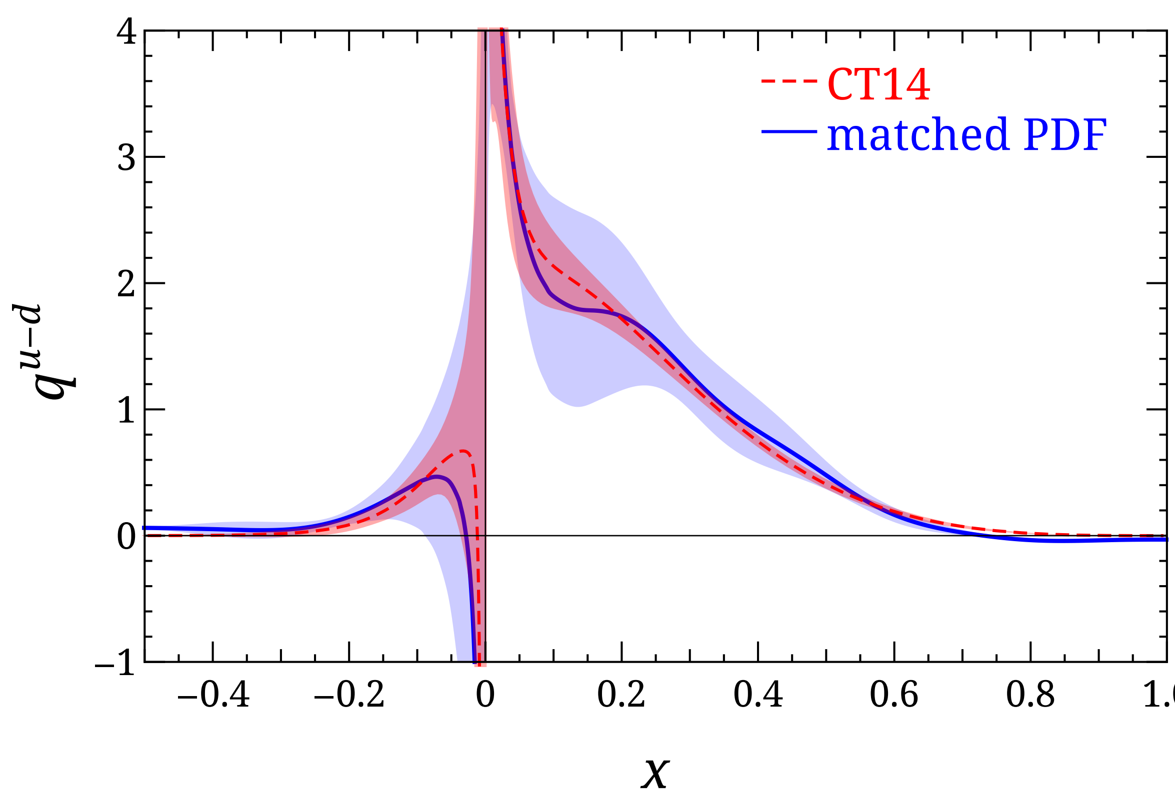


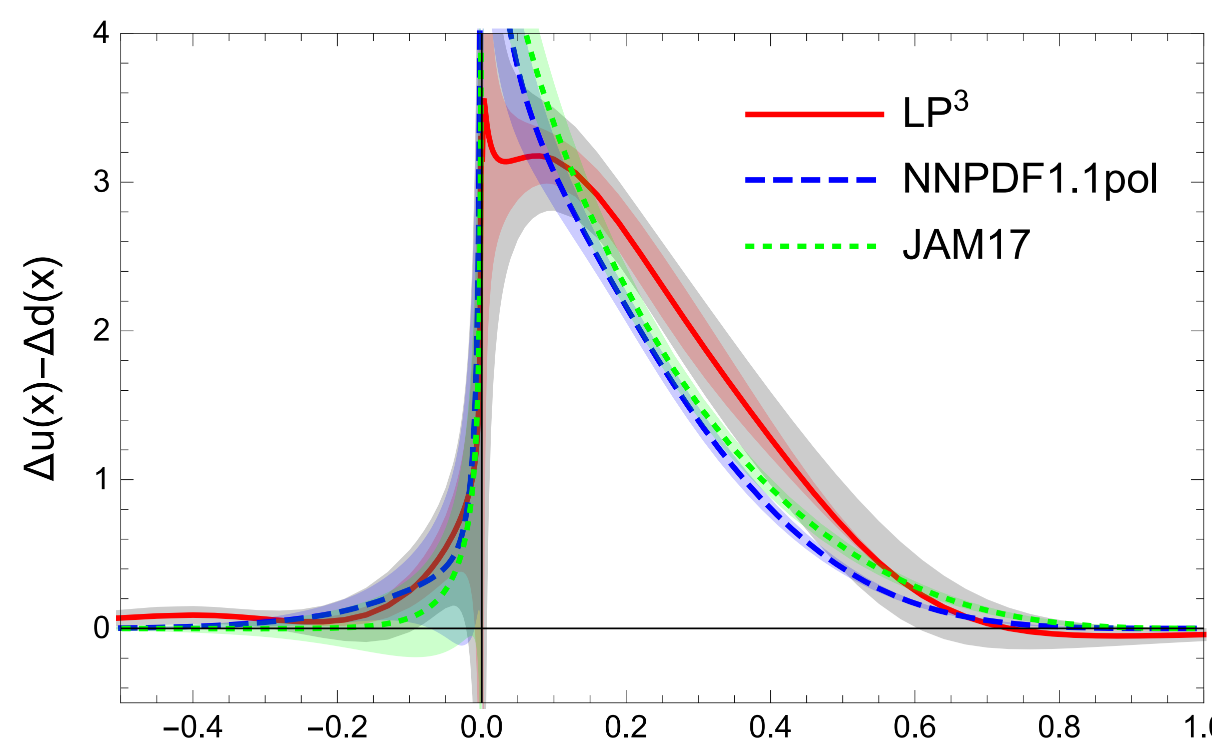
Parton Distribution Functions

- Any improvement benefits LHC searches.
- Key measure of nucleon structure.
- Explosion of numerical & theoretical work ⇐ 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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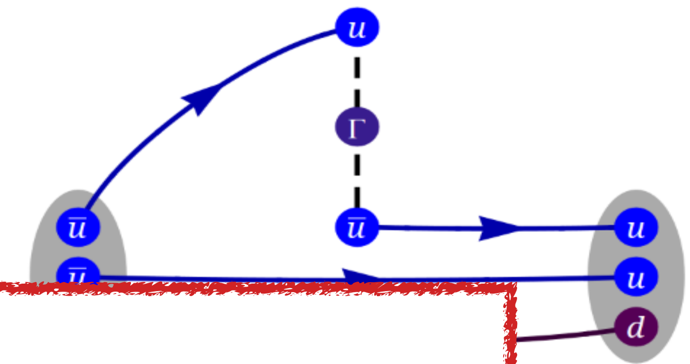
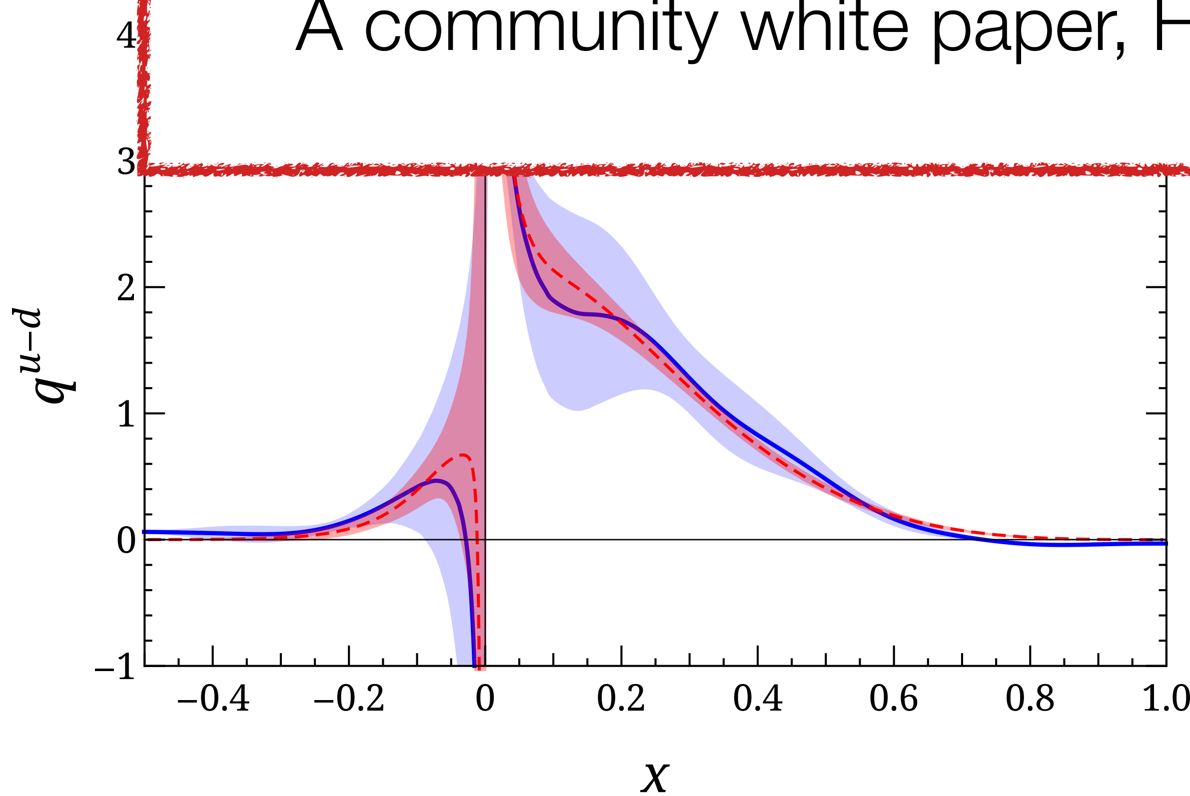
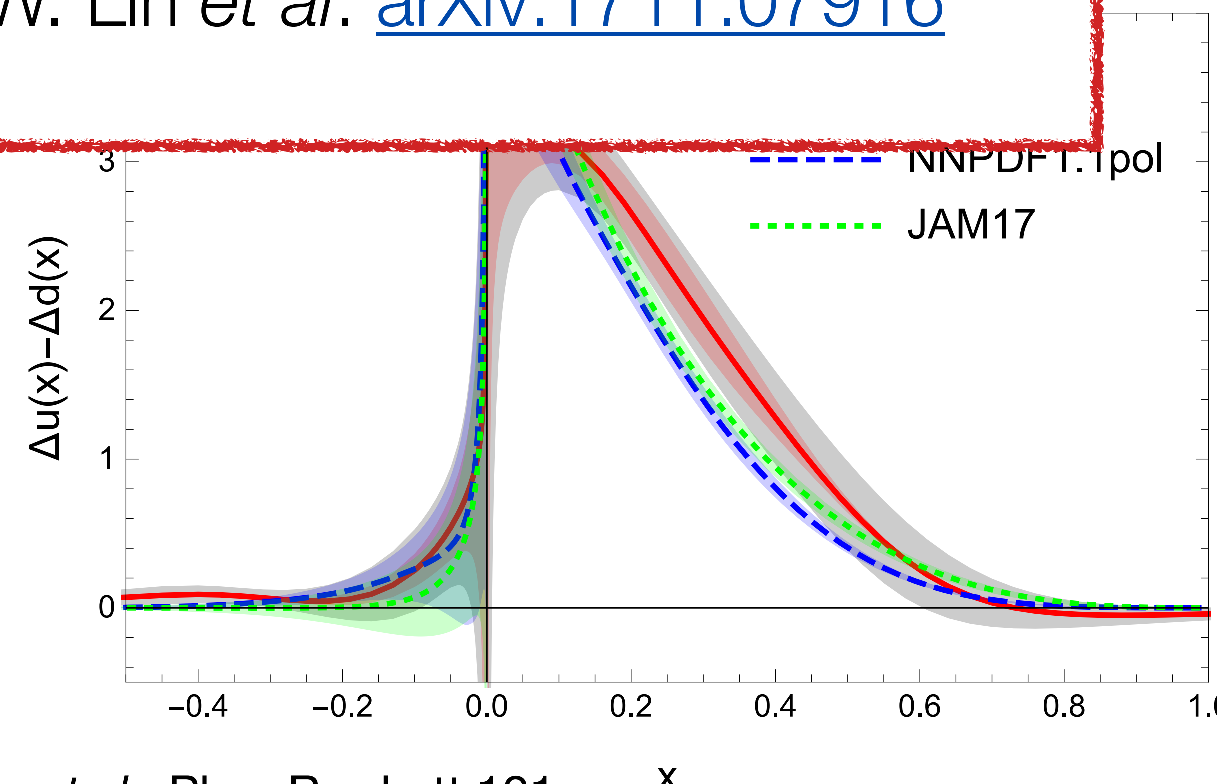


Parton distributions and lattice QCD calculations:
A community white paper, H.-W. Lin *et al*. arXiv:1711.07916

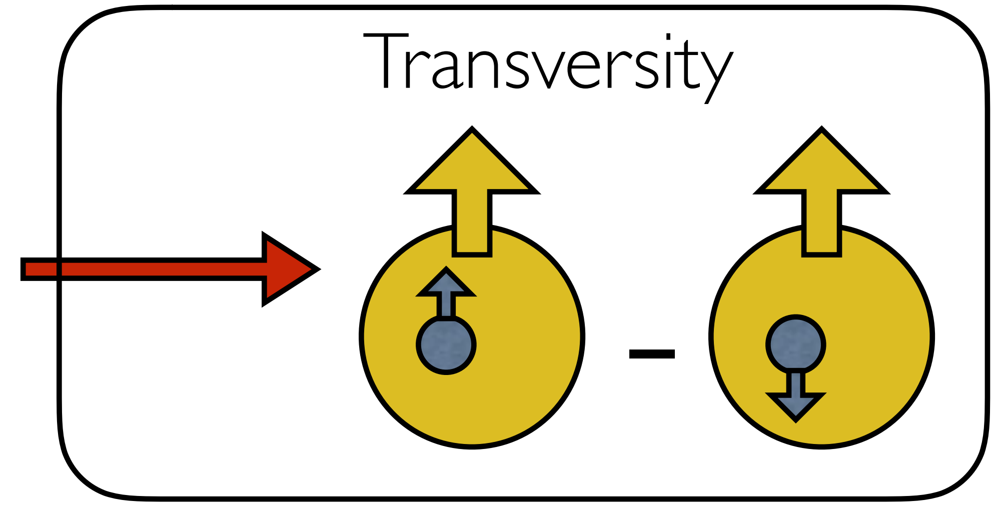


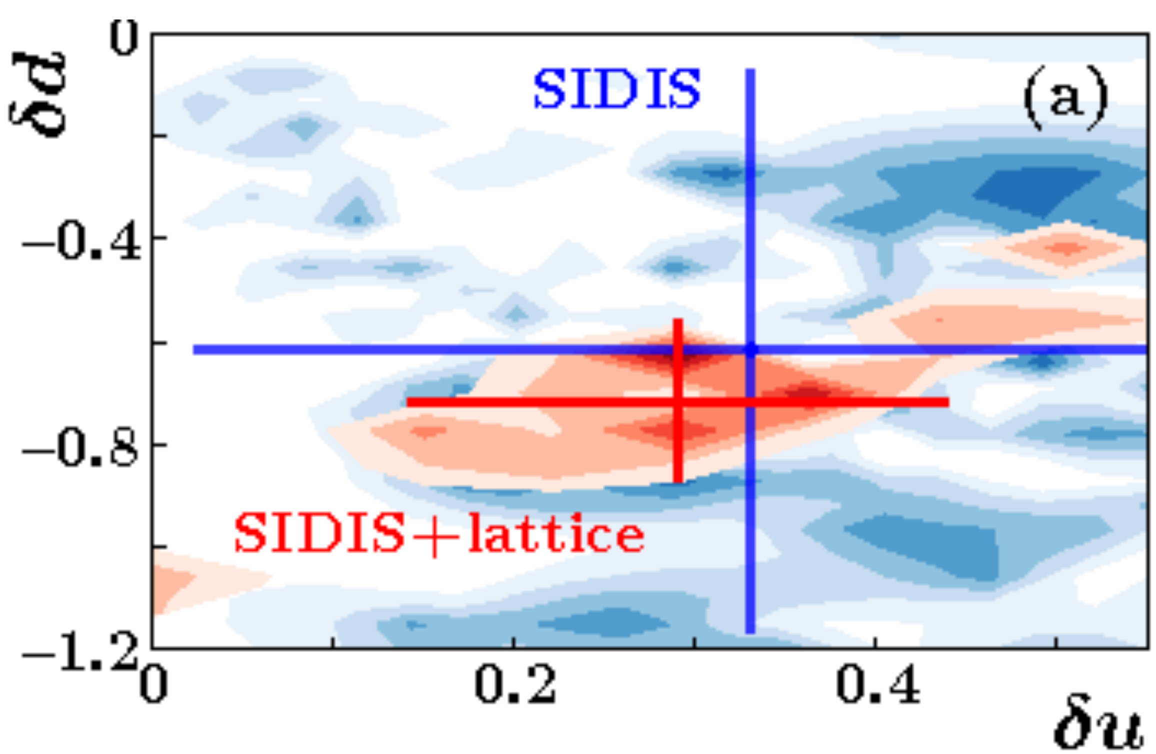


Chen *et al*., arXiv:1803.04393; Lin *et al*., Phys.Rev.Lett 121

Nucleon Structure

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

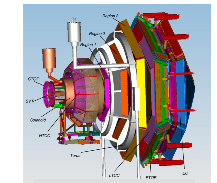




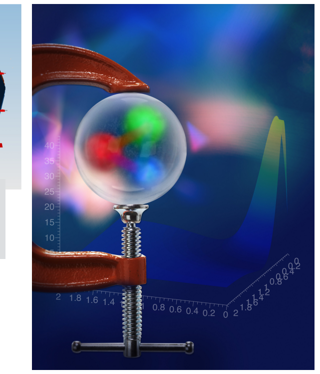
- New global analysis including lattice-QCD constraints:
  - Lin, et.al., Phys.Rev.Lett 120 (2018)
- Lattice QCD can contribute in many areas of nucleon structure.

Pressure in the proton

Pressure of quark/glue mapped in expt.

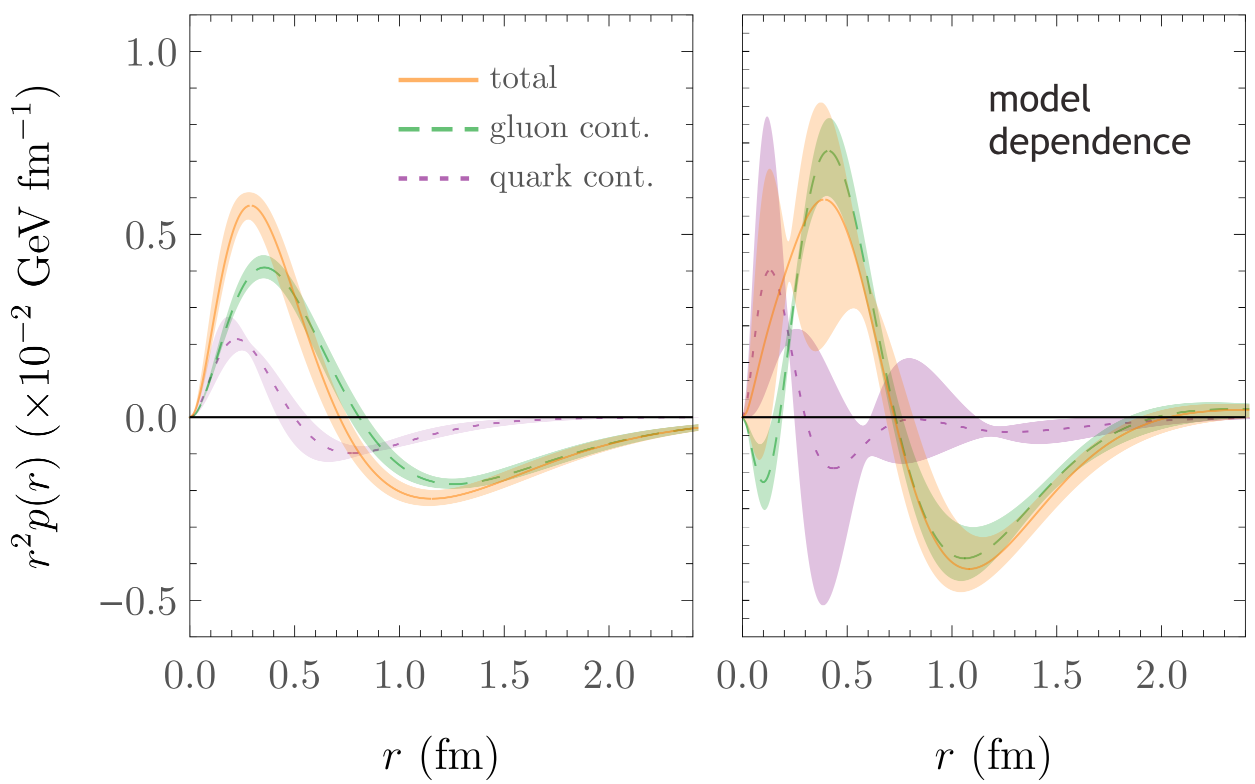


CLAS6

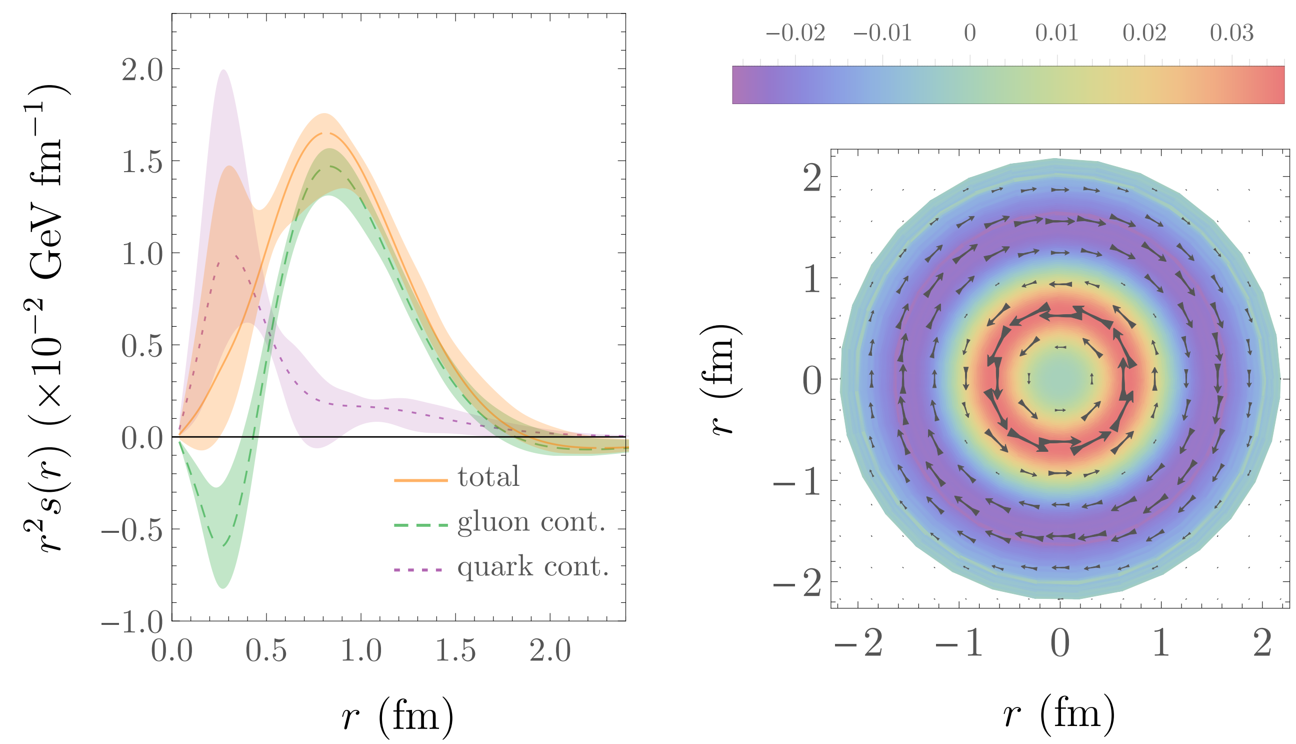


LQCD can compute Energy-Mom. Tensor matrix elements

r^2 * pressure



r^2 * shear



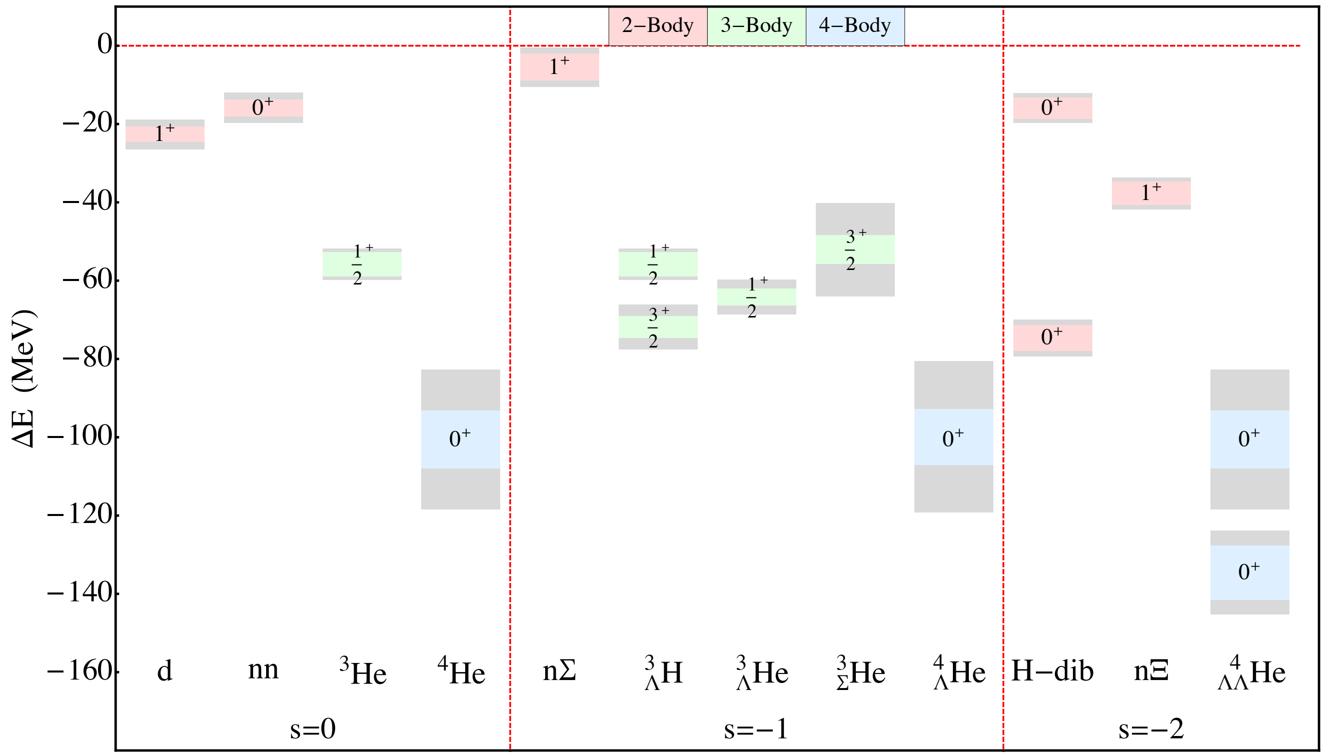
quarks/glue repulsive at core; attractive at boundary

glue lurks near boundary

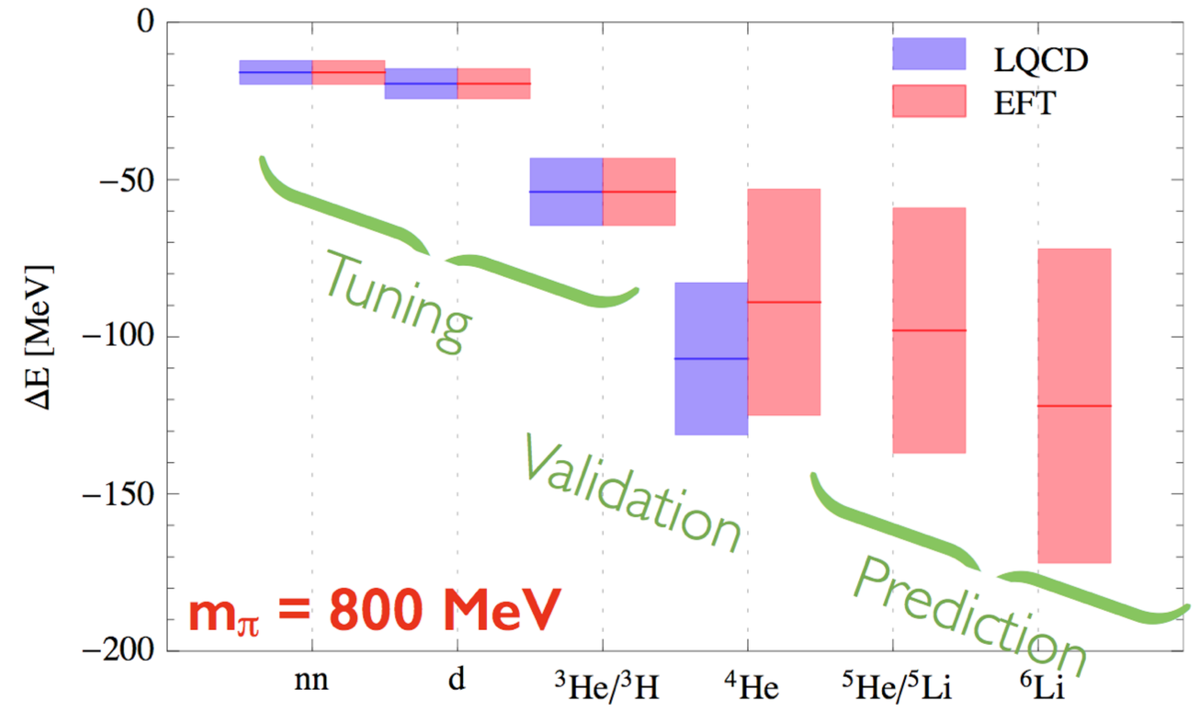
PRL122, 072003 (2019)

QCD for nuclei - milestone

The binding energies of light nuclei+strange nuclei



Nuclear Structure



Refining Nuclear Forces

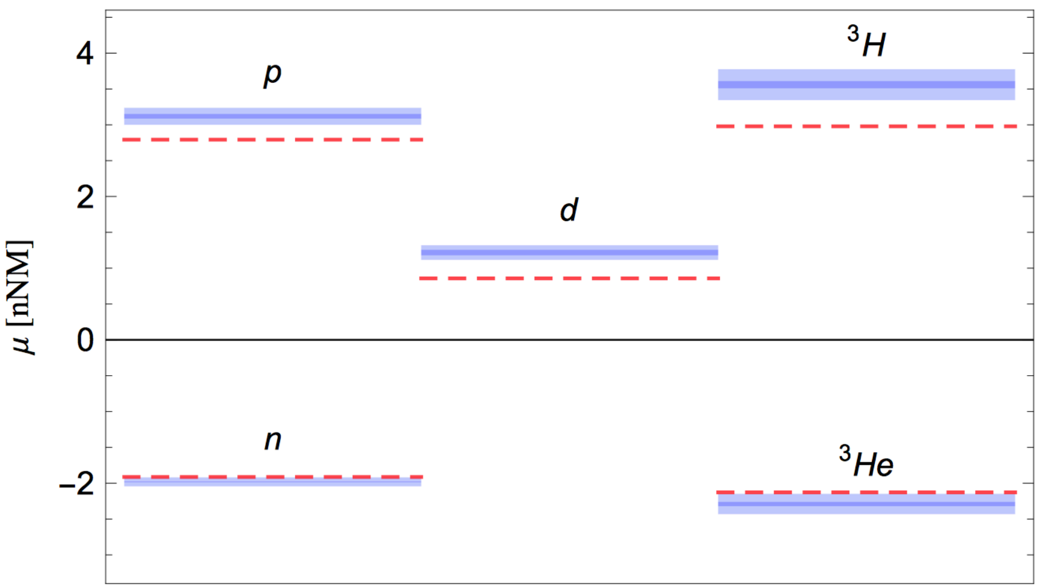
"Effective field theory for lattice nuclei",
PRL 114 052501 (2015)

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

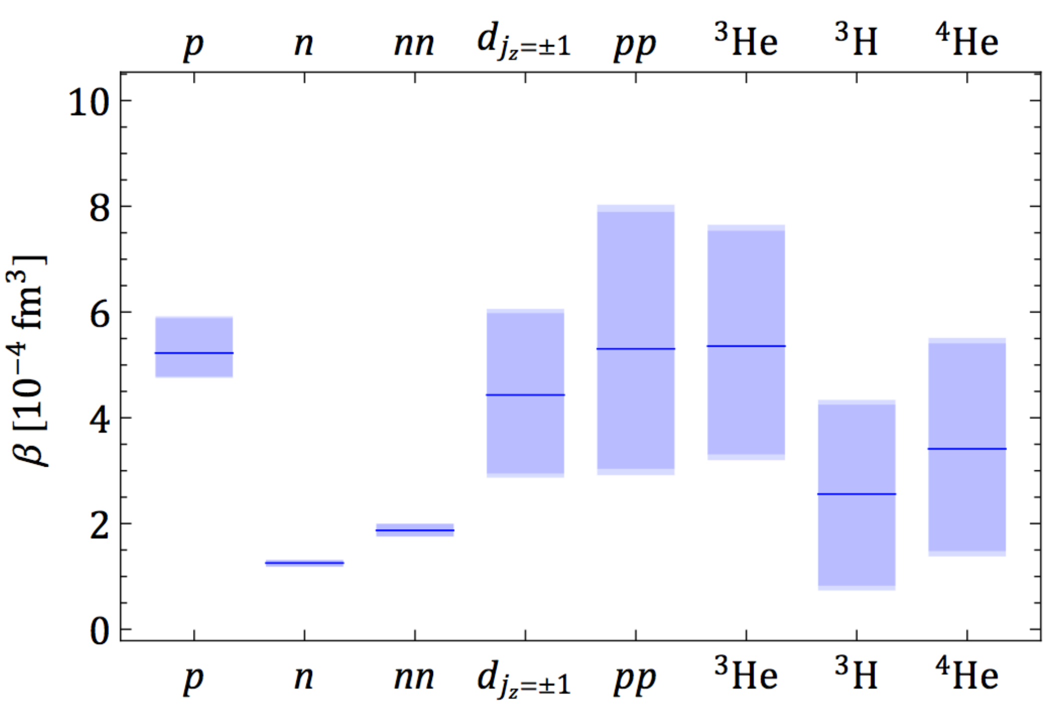
\`Light nuclei and hyper nuclei from QCD in the limit of SU(3) flavor symmetry'
PRD 87 034506 (2013)

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 ββ decay



$M_\pi = 800$ MeV

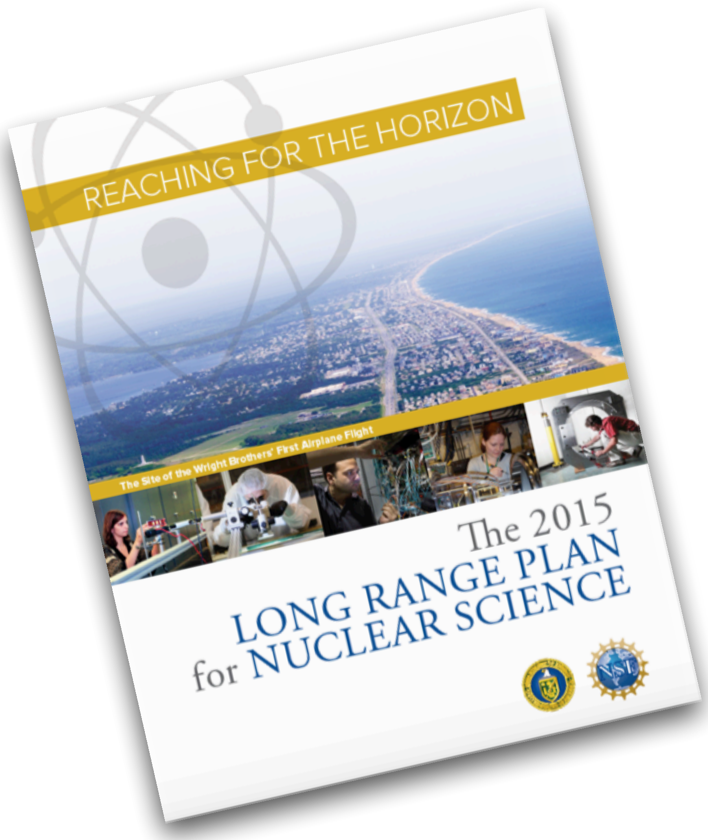


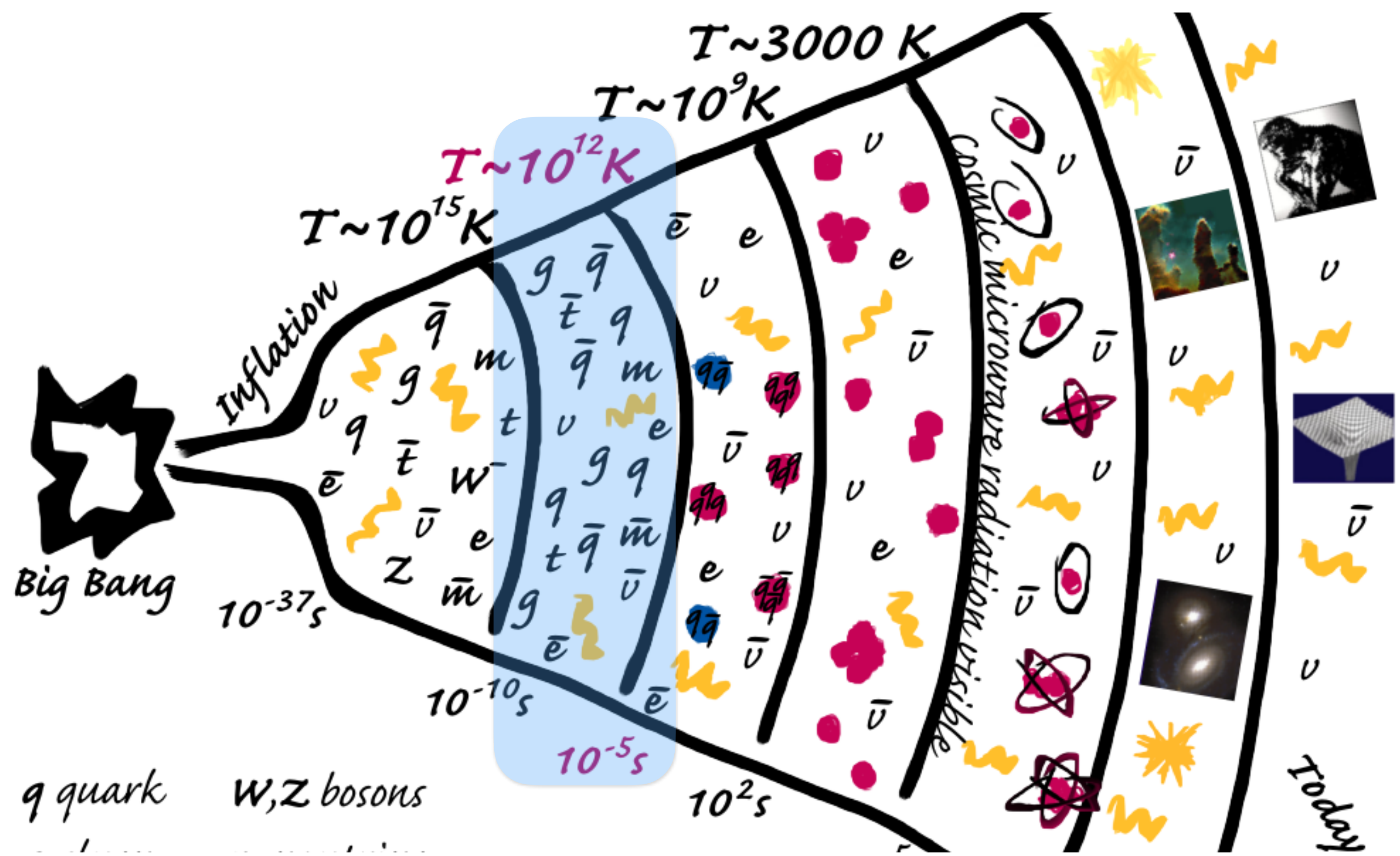
Beane, *et al.*, Phys.Rev.Lett.113 (2014); Tiburzi, *et al.*, Phys.Rev.D96 (2017)

Hot-Dense matter

properties of quark gluon plasma (QGP)

the big questions …



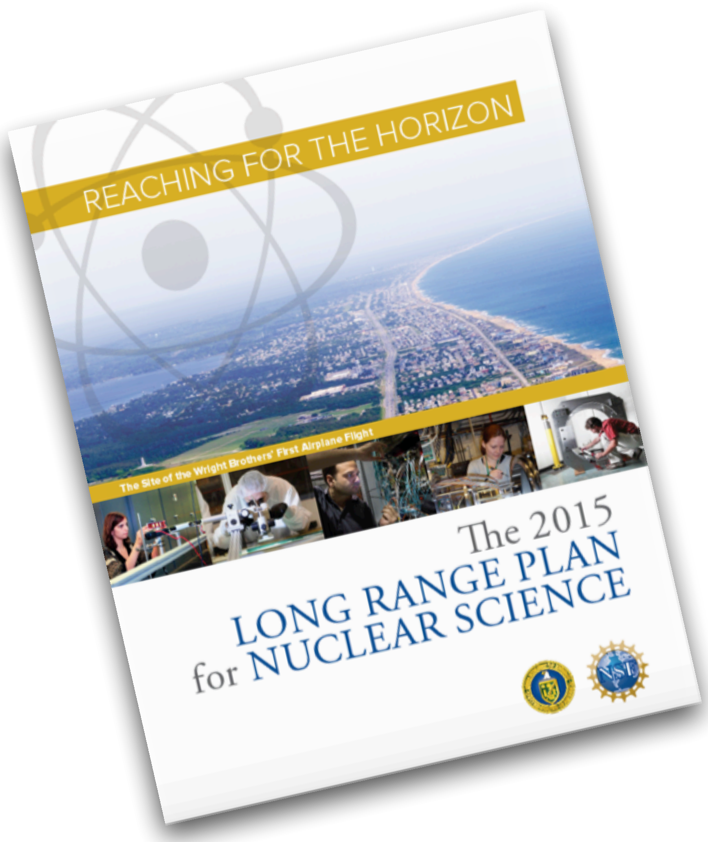


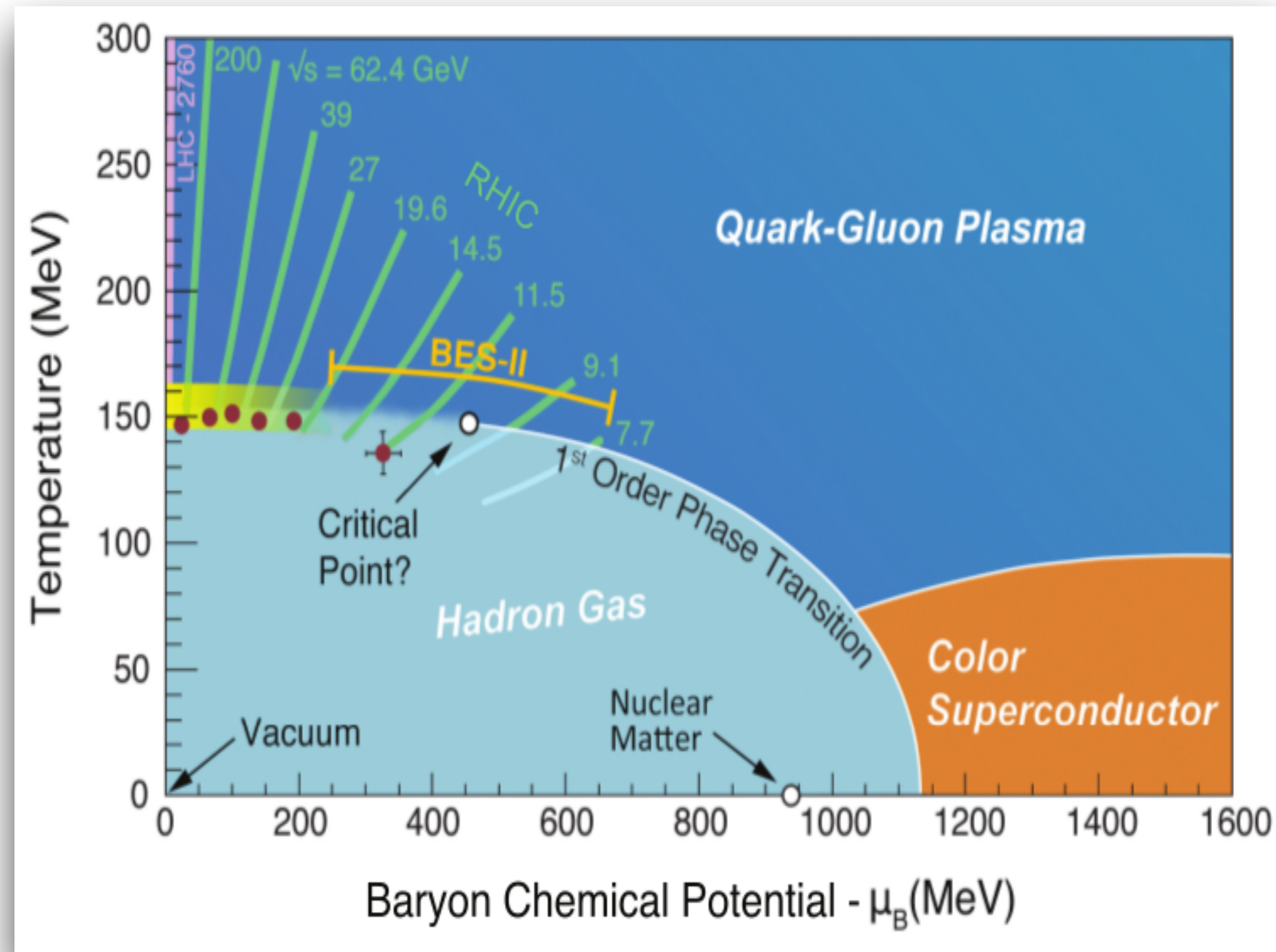
characterize the matter that existed
~ micro-seconds after the Big Bang

Hot-Dense matter

properties of strongly interacting matter

the big questions …





- varying temperatures and densities

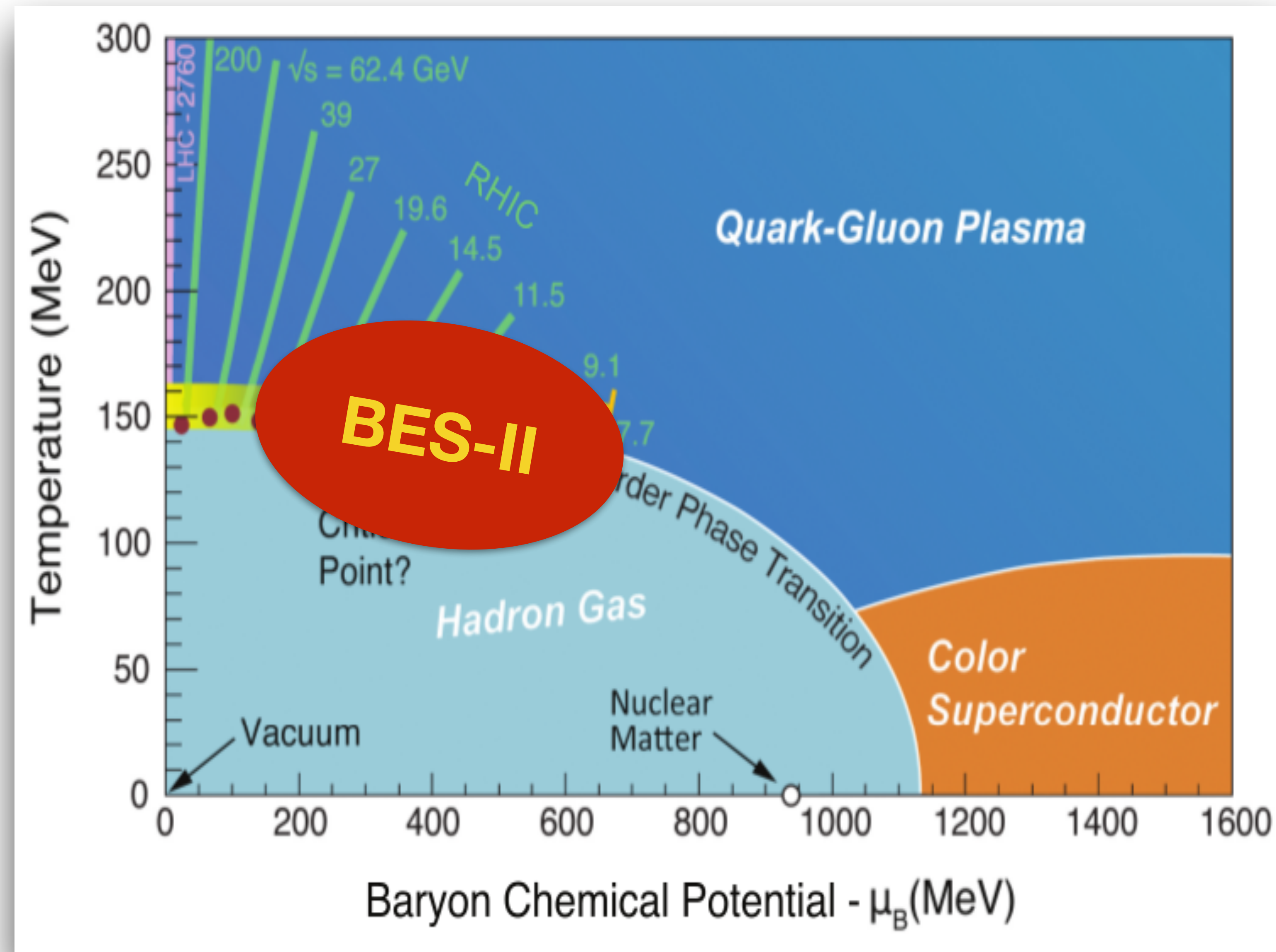
Hot-Dense matter - new expt. at BNL

Beam Energy Scan-II @ RHIC

STAR

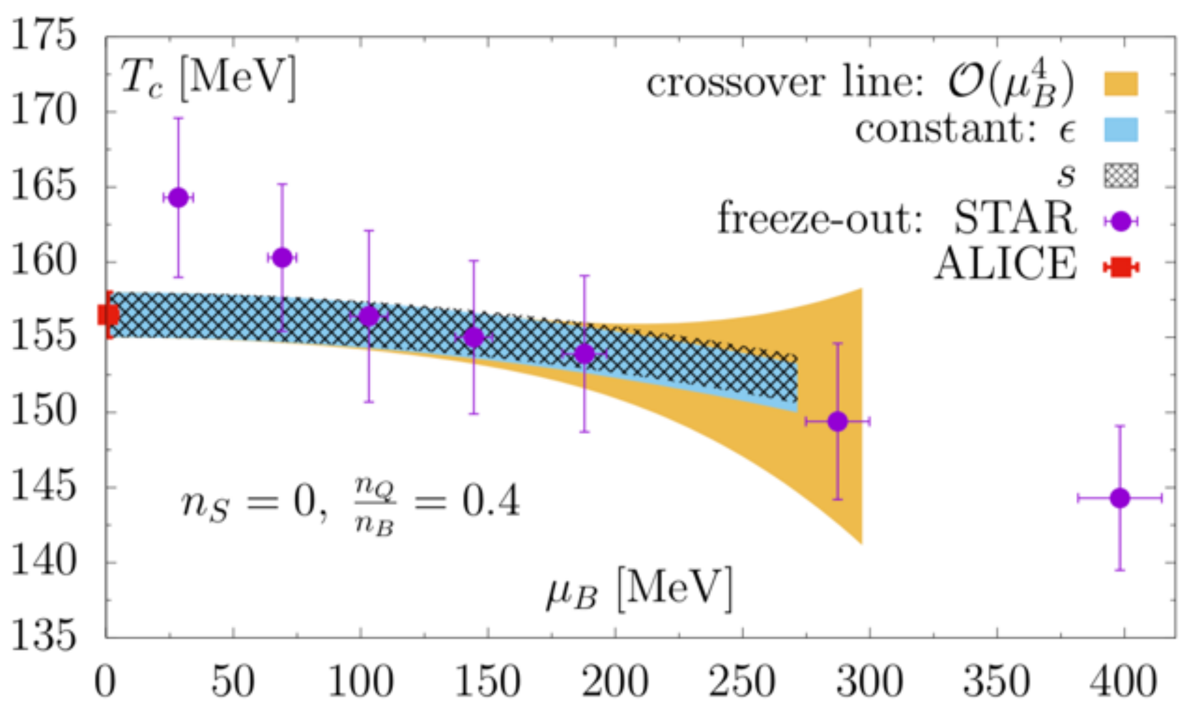
2019-2021

Phase diagram? Critical point?

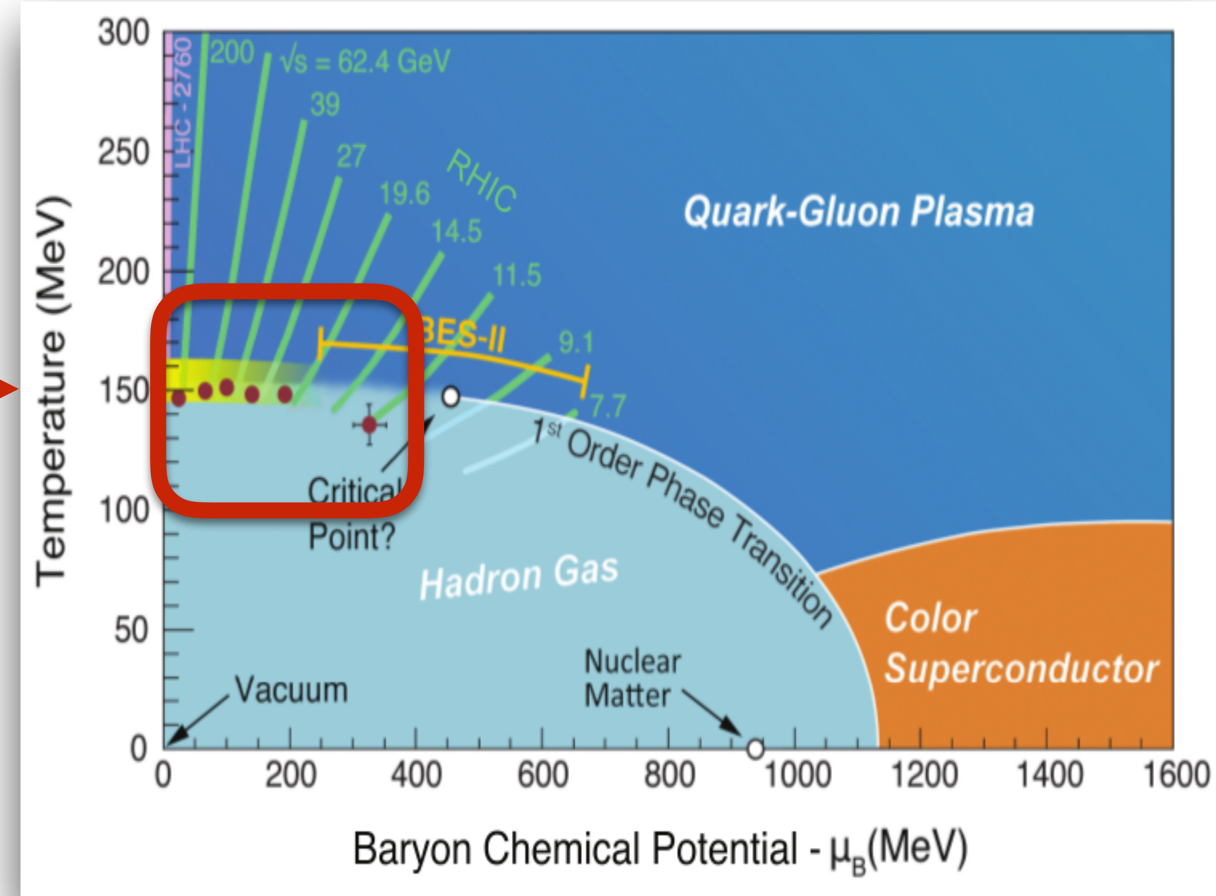


QCD phase boundary computed

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

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

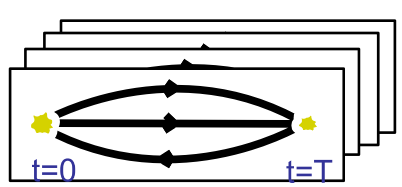
Data-parallel code gen. with comms

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

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

Contractions

Correlators
- O(1M)/cfg

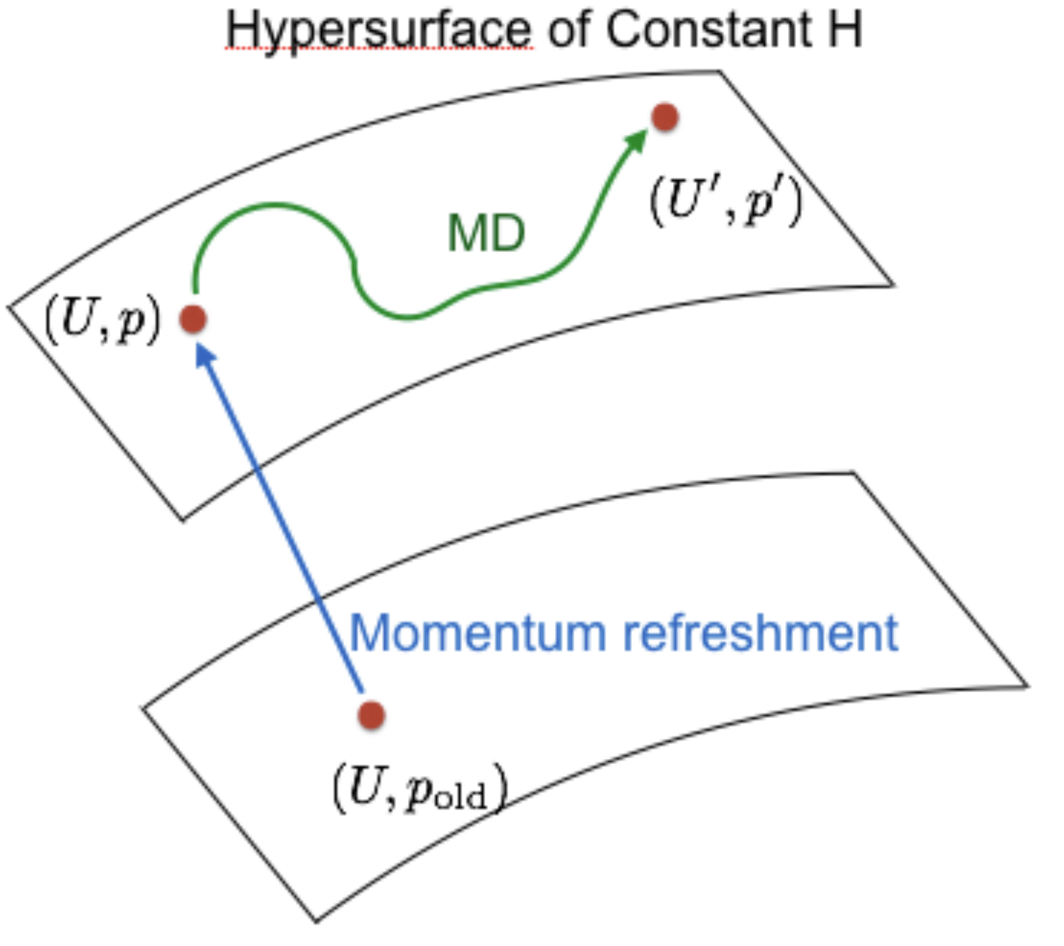


“Workflow” challenge
- Combinatorics -> improved graph theoretic methods
- Code generation for (sparse?) tensor contractions
- Job coordination -> Grid based

How to produce gauge fields?

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

- Limitations



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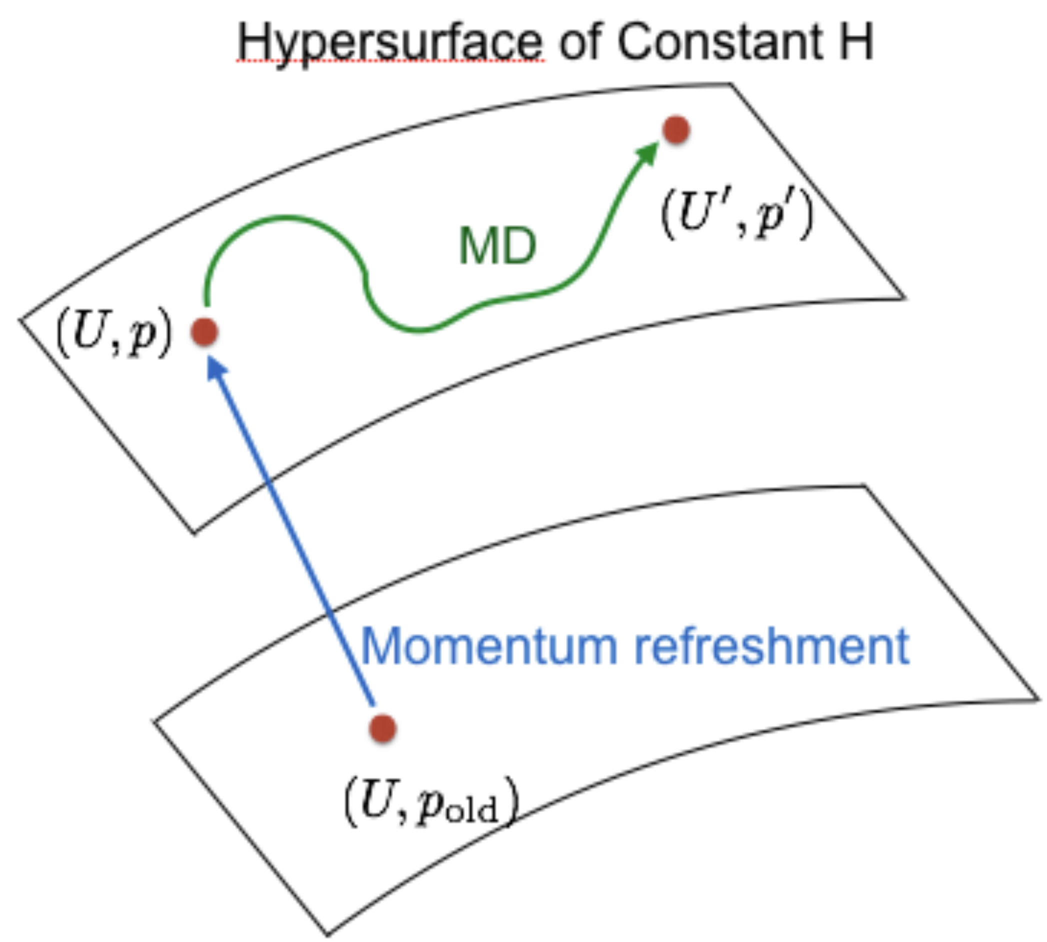
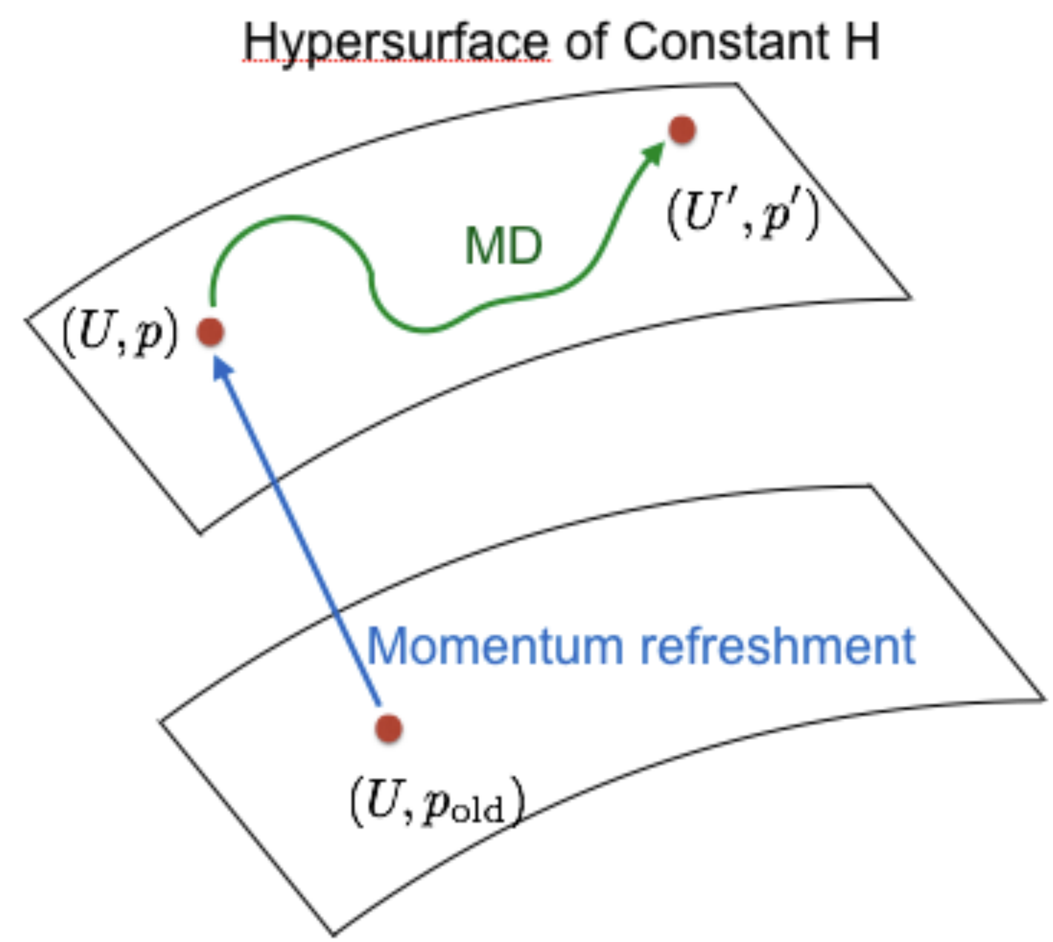
- Limitations
  - Must be "reversible"



How to produce gauge fields?

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

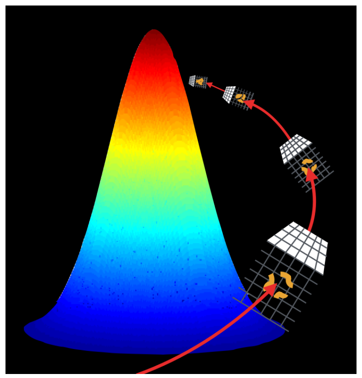
- Limitations
  - Must be "reversible"
  - No adaptive time steps

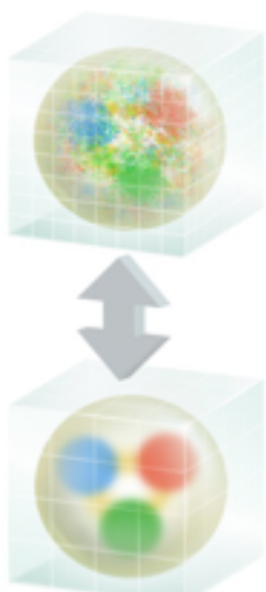


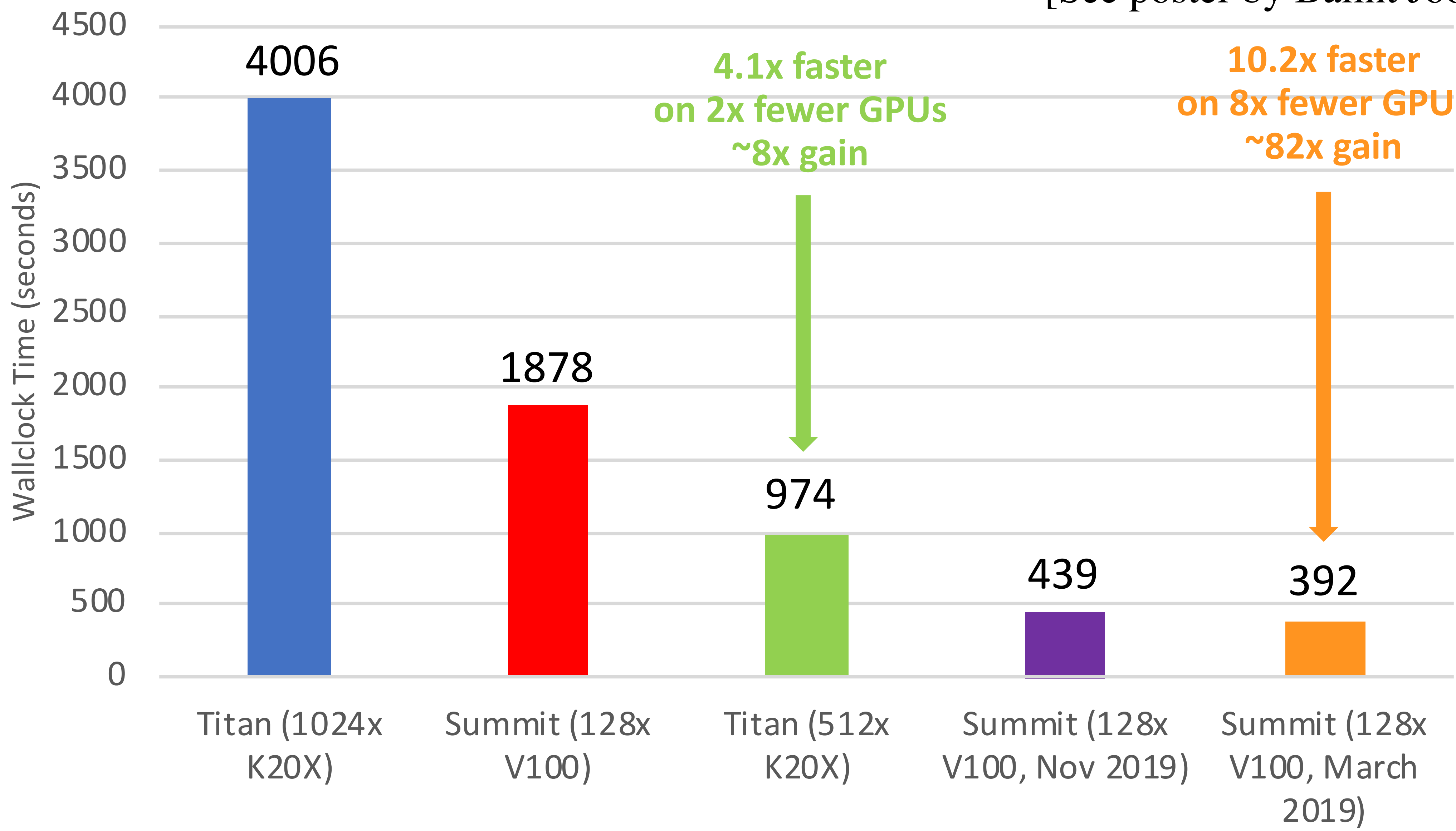
Accelerating QCD gauge generation on GPUs

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 “thoughput”

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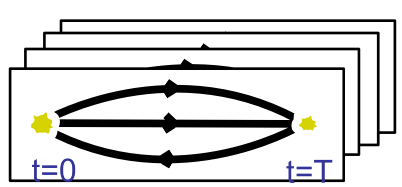

“Workflow” challenge
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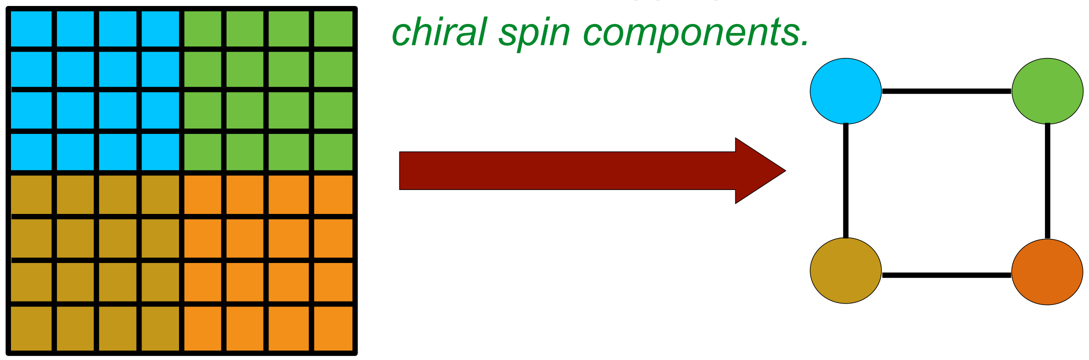
Accelerating propagators

[See poster by Balint Joo]

Collaboration involving ASCR support and Industry partners

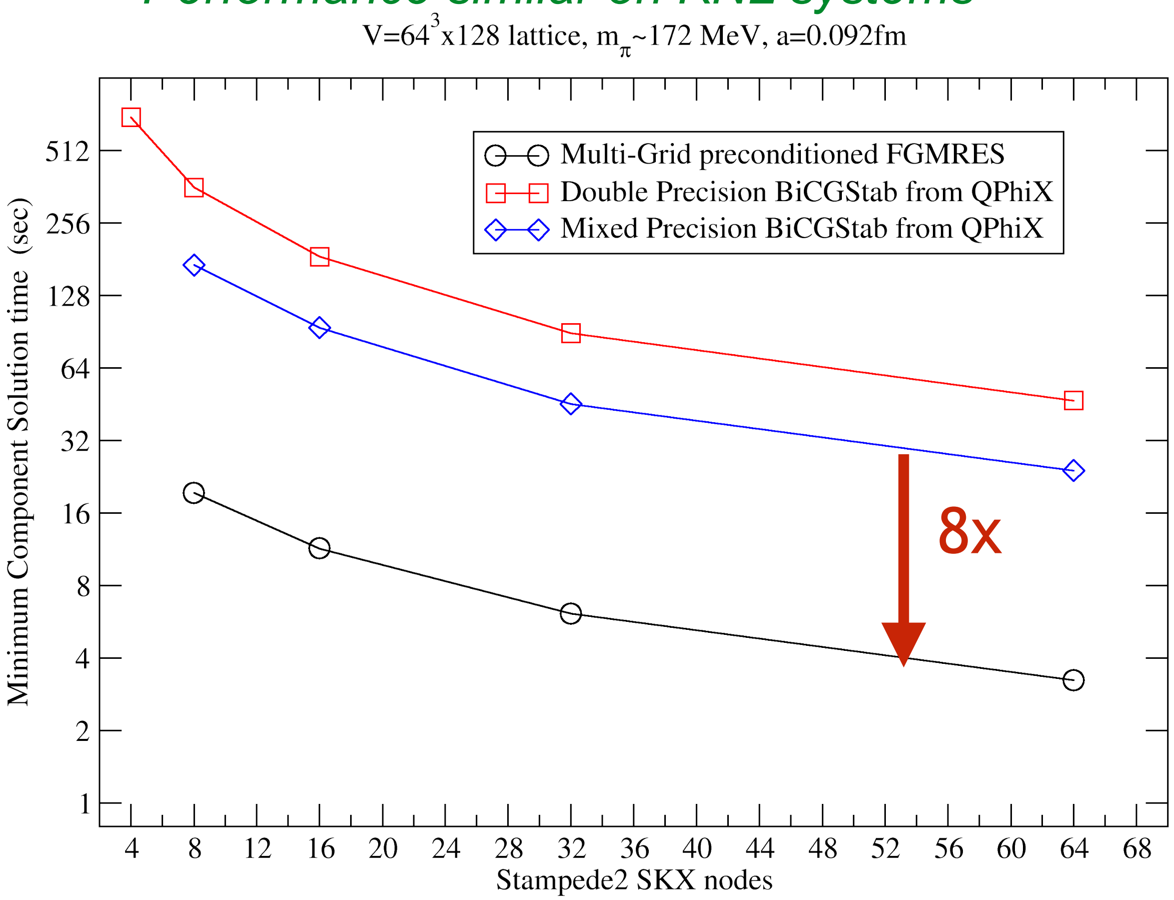
- O(1M) right-hand sides for Dirac equation per configuration
- Ill-conditioned solver at light quark masses
- Solution - Adaptive Multigrid

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



Stampede 2 (Skylake) - Strong scaling

Performance similar on KNL systems



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

Happy times on Cori-KNL

Reducing contraction/correlator costs

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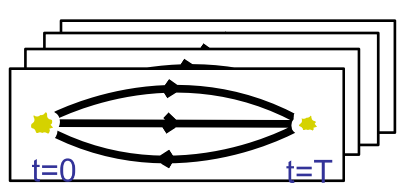

"Workflow" challenge
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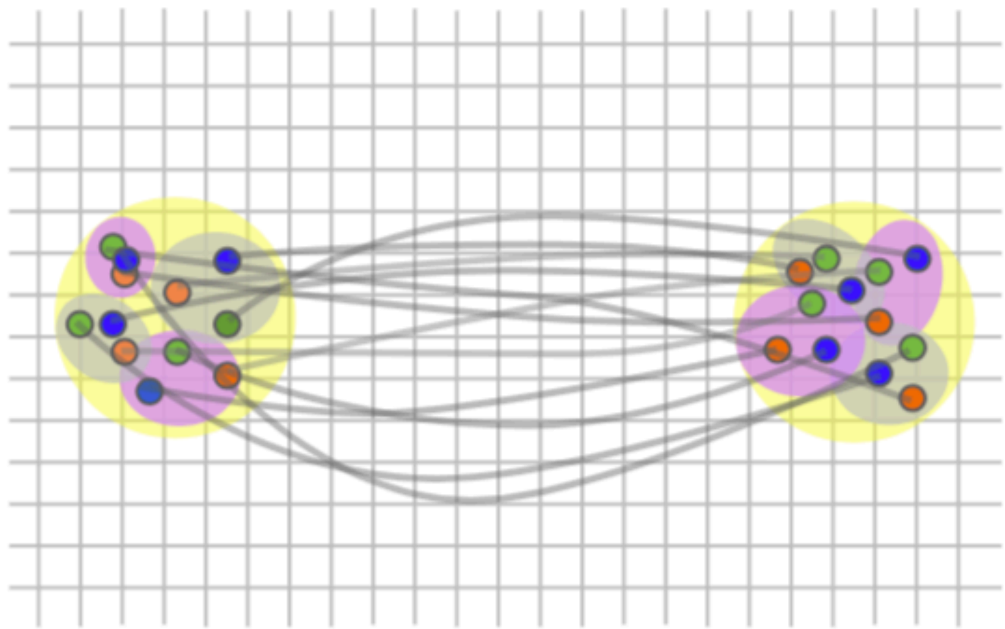
QCD for nuclei

Collaboration involving ASCR support and Industry partners

- Quarks need to be tied together in all possible way

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

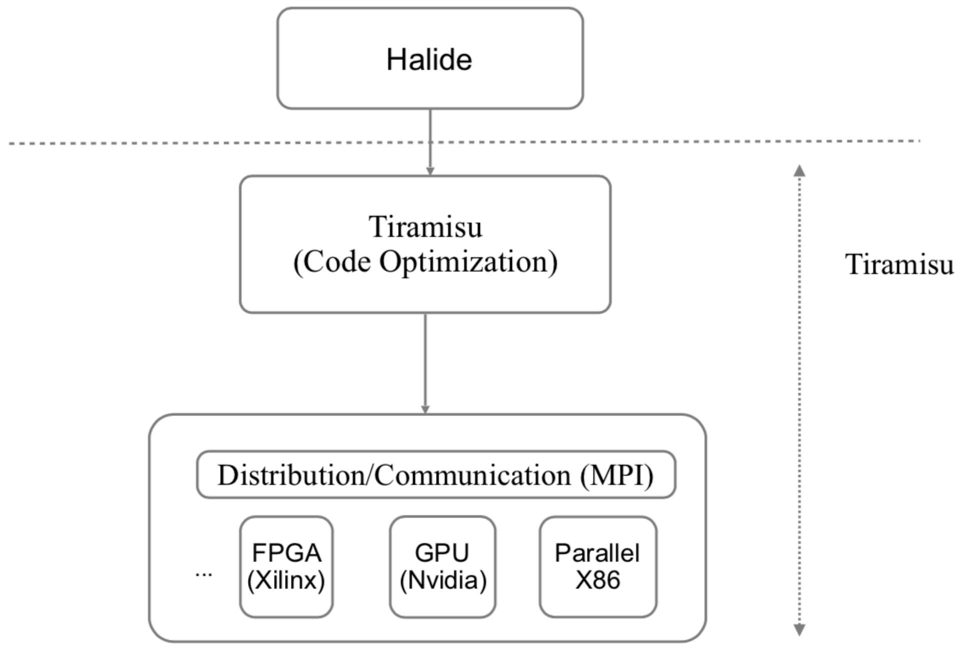


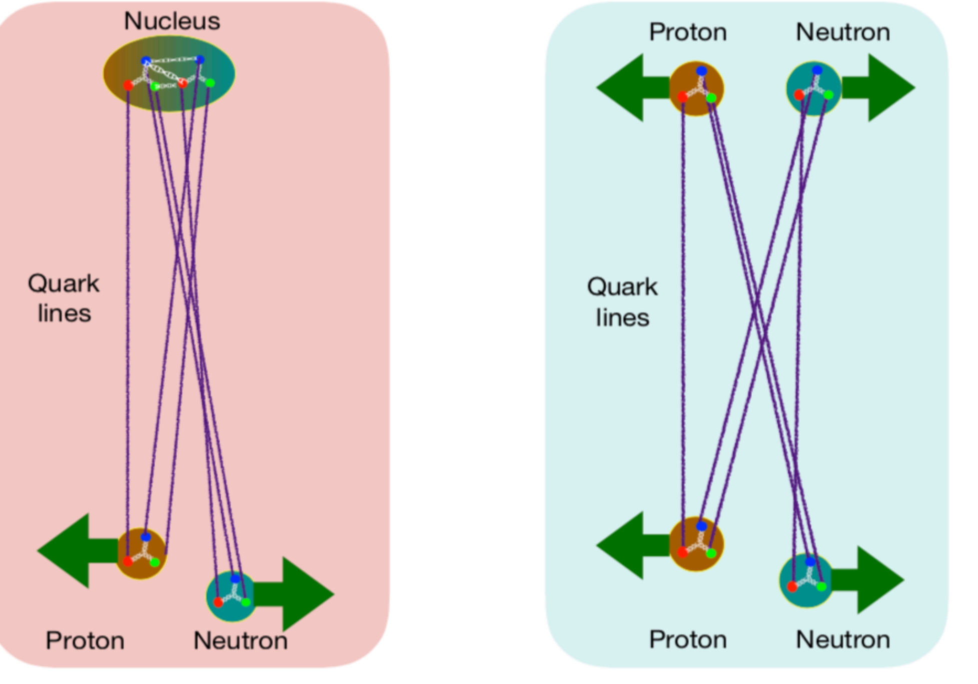
- Manage using algorithmic trickery - still significant graph contractions
- TACO @ MIT (cf TCE, Cyclops) http://tensor-compiler.org
  - general purpose tensor contraction compiler framework
  - target to QCD specific problems (sparsity patterns, …)
  - Allow efficient exploration of methodology

QCD for nuclei - Halide & Tiramisu

- Extend Tiramisu to accomodate LQCD & CUDA

[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

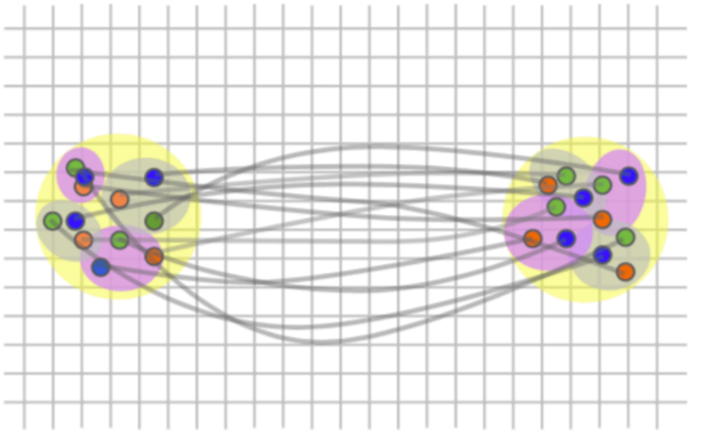
QCD for nuclei - going to physic quark masses

- Reduce the volume scaling cost by reducing the volume!

[See poster session]

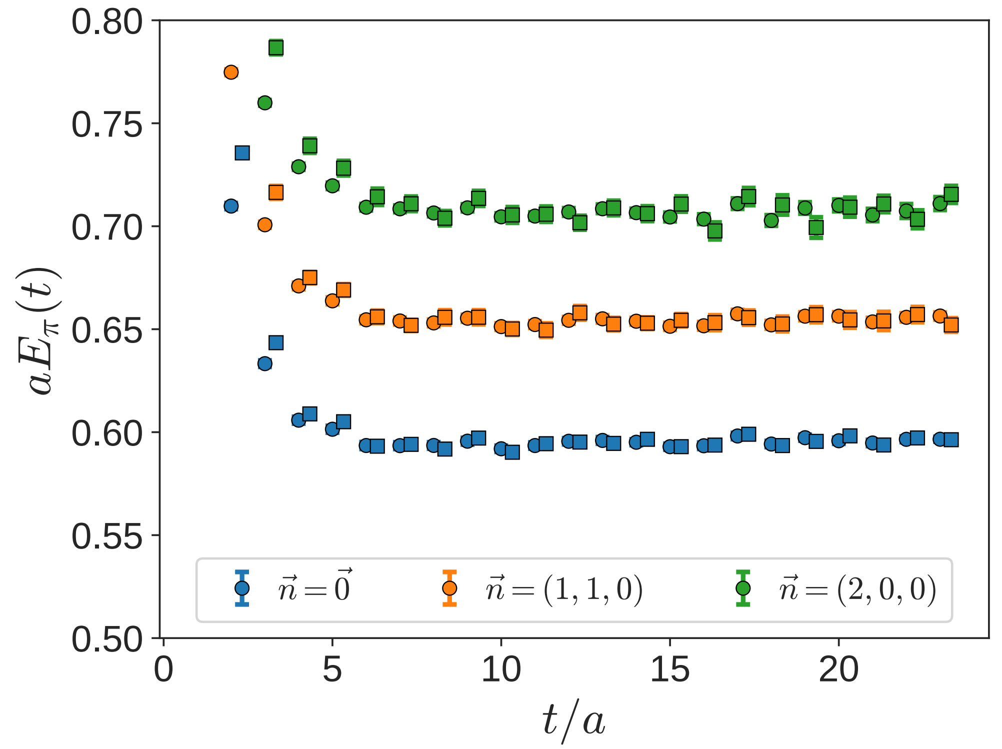
Restriction: Aggregation over sites

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



- 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

- 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