Lattice QCD in Nuclear Physics

Robert Edwards
Jefferson Lab

CCP 2011

What is this?

What is this?

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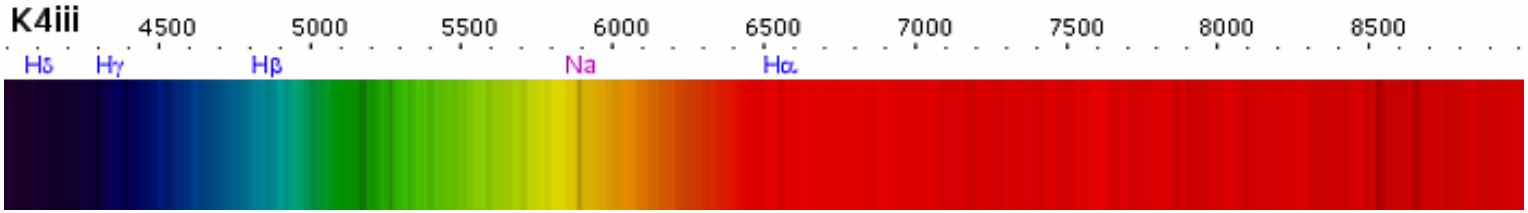
K4iii
4500
5000
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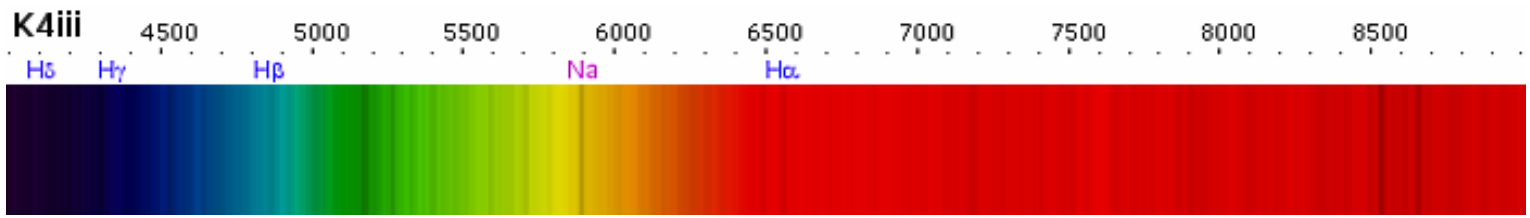
Hδ
Hγ
Hβ
Na
Hα

What is this?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Spectroscopy of QCD

Spectroscopy reveals fundamental aspects of hadronic physics

- Essential degrees of freedom?
- Gluonic excitations in mesons - exotic states of matter?

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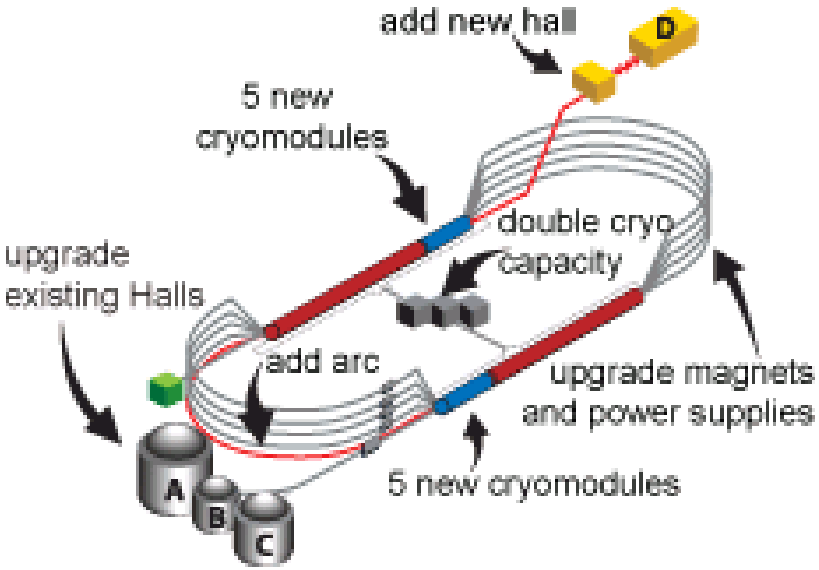
- New spectroscopy programs world-wide
  - E.g., BES III (Beijing), GSI/Panda (Darmstadt)
  - Crucial complement to 12 GeV program at JLab.
    - Excited nucleon spectroscopy (JLab)
    - JLab GlueX: search for gluonic excitations.

Nuclear Physics & Jefferson Lab

JLab undergoing a major upgrade



Future Hall D

- **Lab doubling beam energy to 12GeV**
- **Adding new experimental Hall**

USQCD National Effort

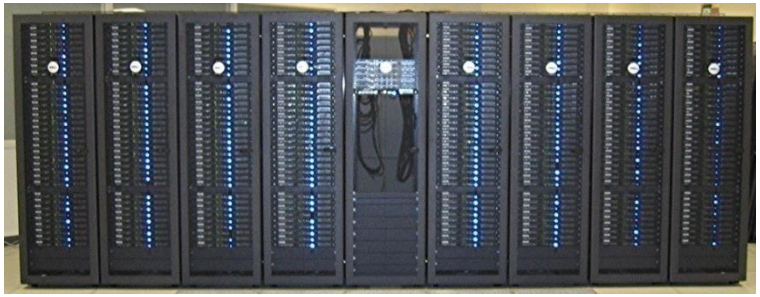
US Lattice QCD effort: Jefferson Laboratory, BNL and FNAL

FNAL
Weak matrix elements

BNL
RHIC Physics

JLAB
Hadronic Physics

SciDAC – R&D Vehicle
• Software R&D



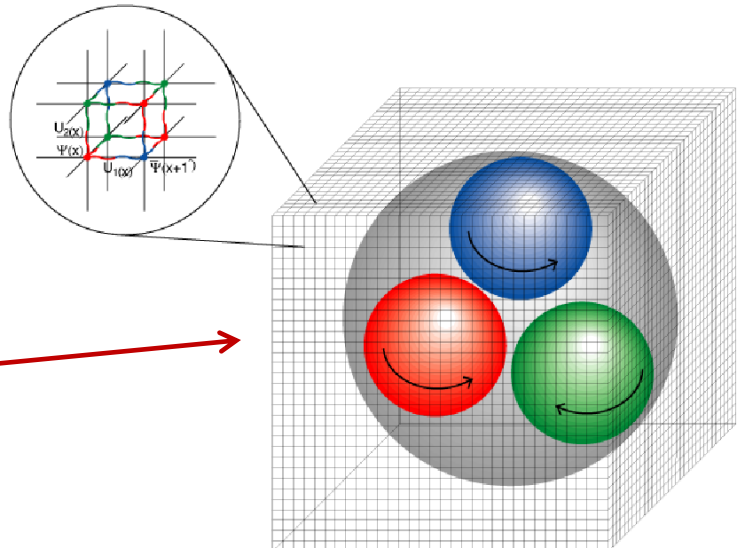
INCITE resources + USQCD cluster facilities:

Impact on DOE's High Energy & Nuclear Physics Program

QCD

- QCD: Dirac operator: A_ν (vector potential), m (mass), γ_ν (4x4 matrices)

$$D(A,m) = -i\sum_{\nu=1}^{4}\gamma_\nu\left(\frac{\partial}{\partial x_\nu} + ieA_\nu(x)\right) + m$$



- Lattice QCD: finite difference

- Probability measure:

$$d\mu = e^{-S(A)}\det(D(A,m_{up}))\det(D(A,m_{down}))\det(D(A,m_{strange}))$$

- Observables:

$$\langle\mathcal{O}\rangle = \int d\mu\,\mathcal{O}(A) \quad \rightarrow \quad \frac{1}{N}\sum_{n=1}^{N}\mathcal{O}(A_n)$$

How to produce gauge fields?

- Hamilton's eq's - 1st order coupled diff. eq's – in a fictitious time

$$H = \frac{1}{2}P^2 + S_{\text{gauge}}(A) + \phi^\dagger \left[D(A)\right]^{-1} \phi$$

Momentum

Energy in gauge fields

Energy in quark fields

- Integrator requirements:
  - Reversible
  - Volume preserving
- Proposals for Metropolis M.C. update

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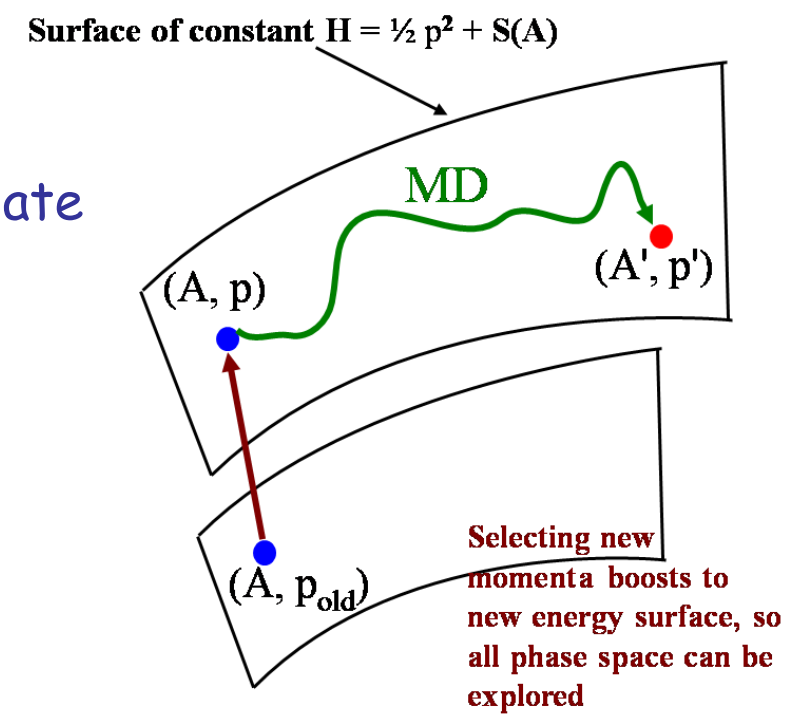

Hamiltonians, integrators, shadows…

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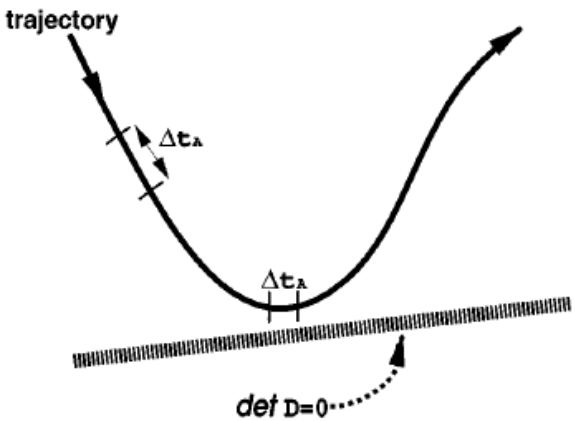
$$H = \frac{1}{2}P^2 + S_{\text{gauge}} + S_{\text{quark}}$$

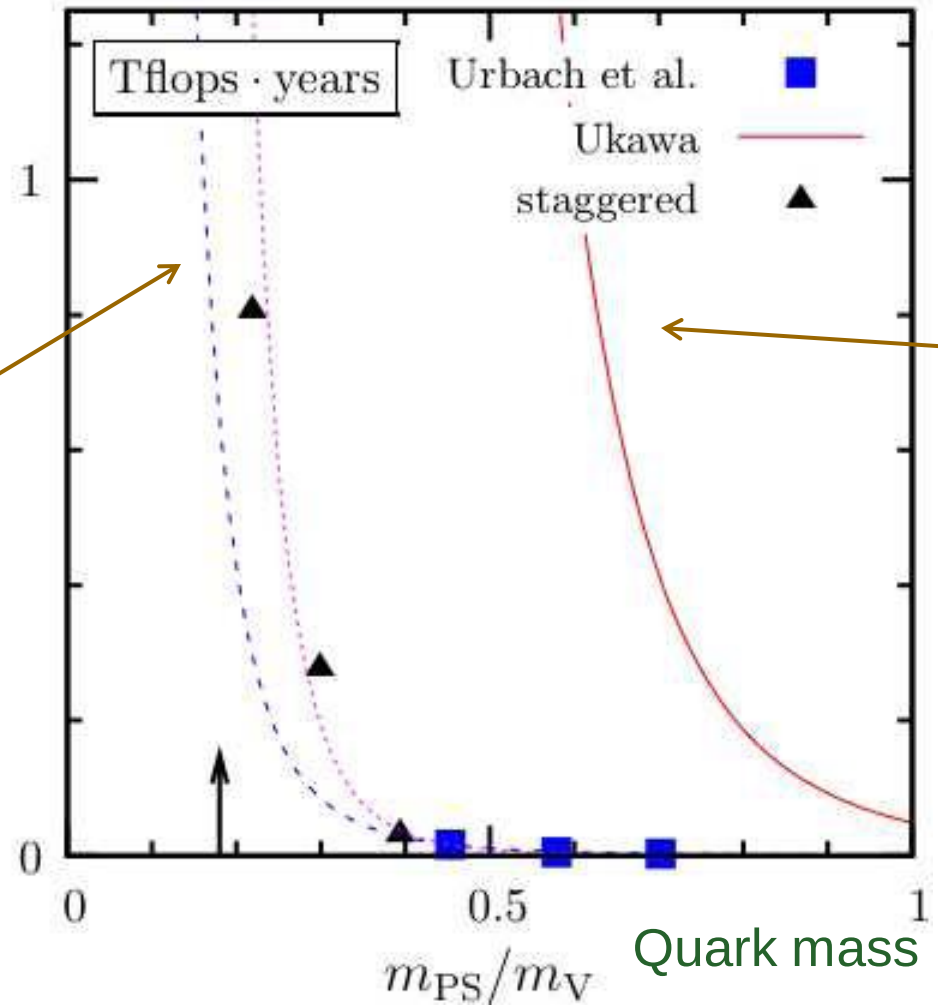


- Integrator tools (very active research area)
  - Symplectic method of choice
  - Update gauge/quark on different scales
    - Balance forces - avoid linear solver calls
  - Different schemes/orders: Leapfrog, Omelyan, etc…,
  - det(D(A)) $\rightarrow$ add/subtract action terms (preconditioning)
- Shadow Hamiltonian techniques:
  - Poisson brackets - optimal integrator tuning parameters

(Using less) "power" with new algorithms

"Berlin" Wall – falling!

Multi-scale integrators, "mass" preconditioning



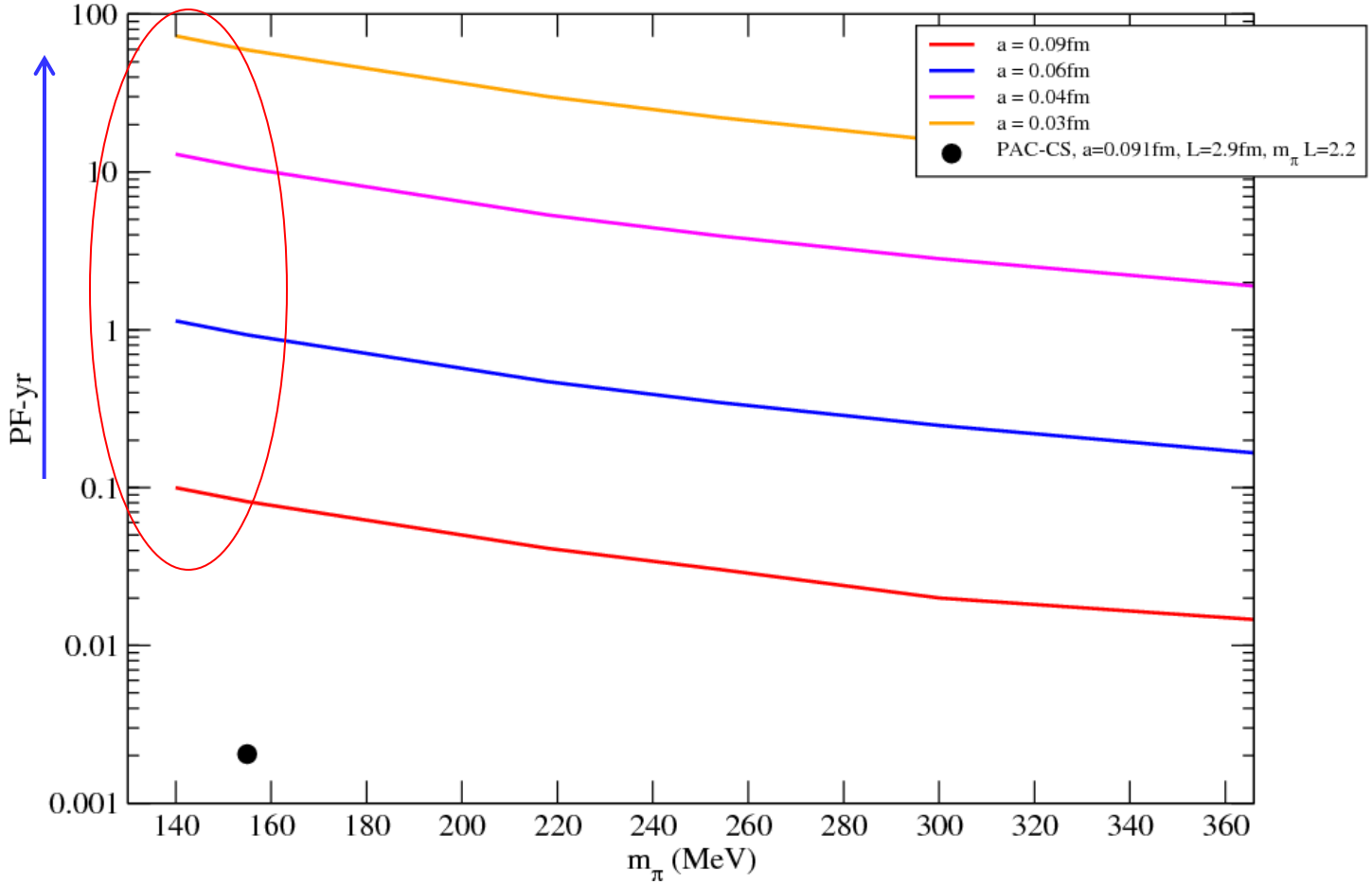
Conventional leapfrog

Quark mass

Gauge Generation: Cost Scaling

- Cost: reasonable statistics, box size and "physical" pion mass
- Extrapolate in lattice spacings: 10 ~ 100 PF-yr

PF-years



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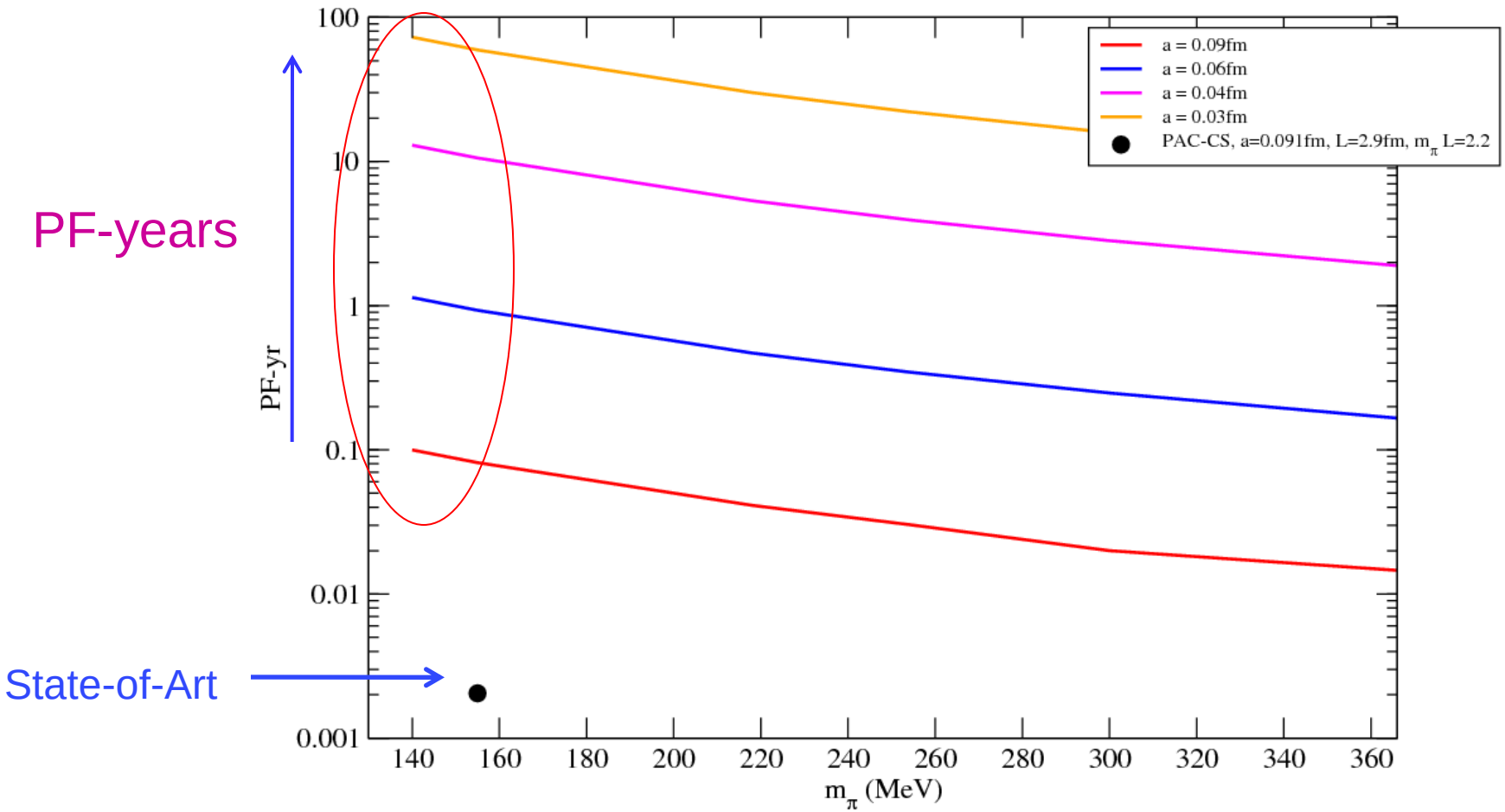

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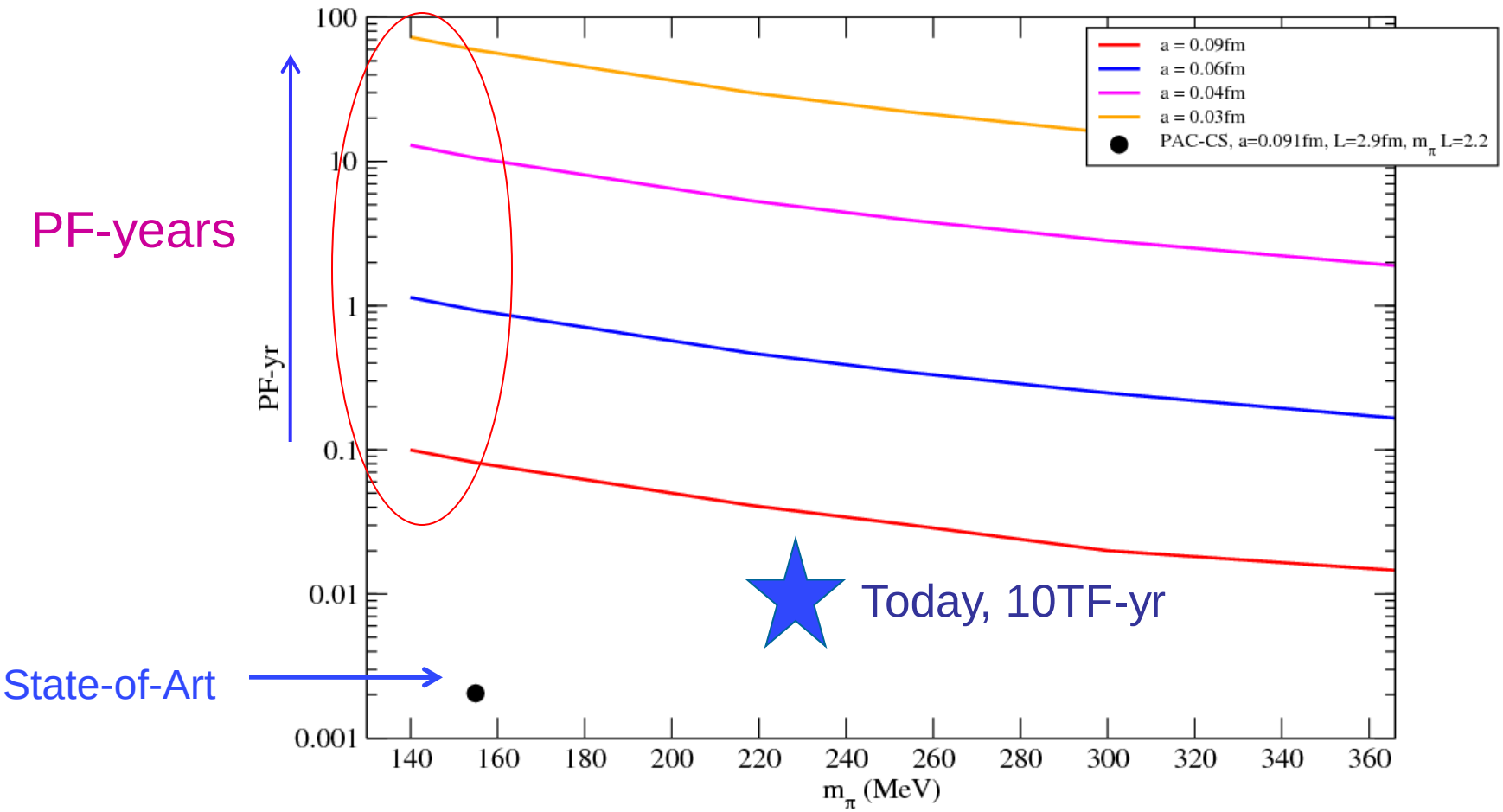

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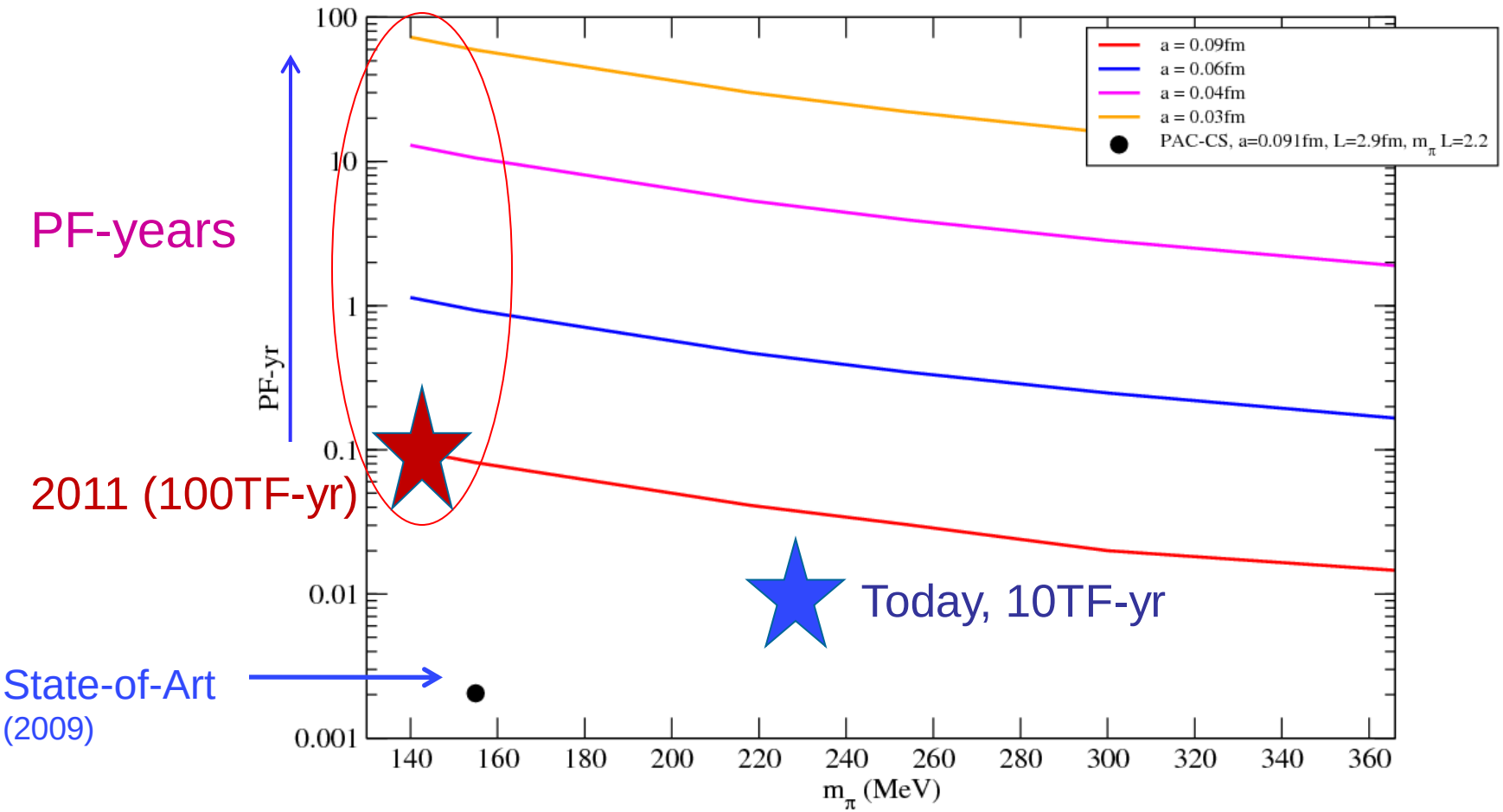

Typical LQCD Workflow

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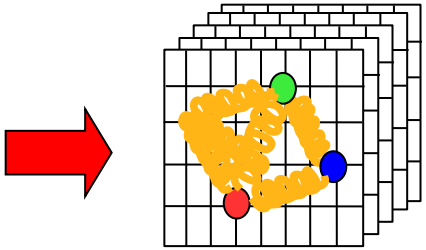
Generate the configurations

- Leadership level
- 24k cores, 10 TF-yr



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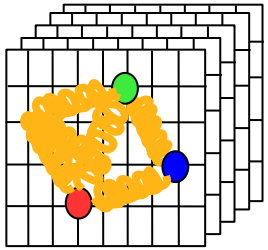
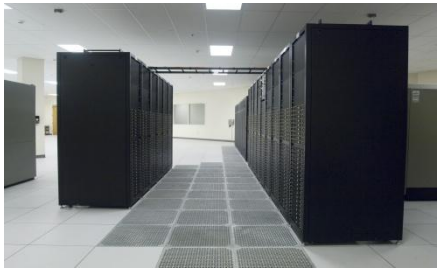
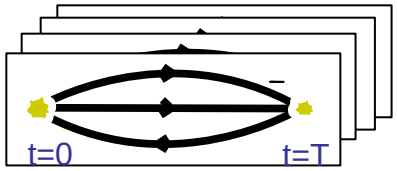




Analyze

Typically mid-range level

256 cores



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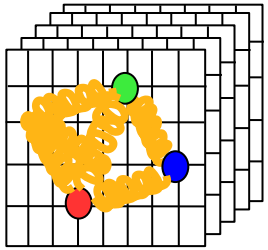

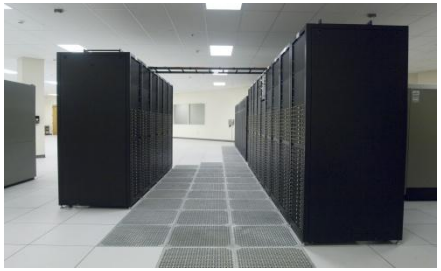

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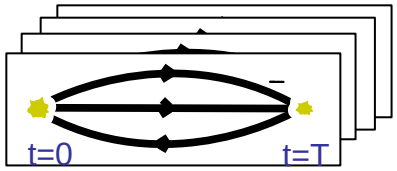

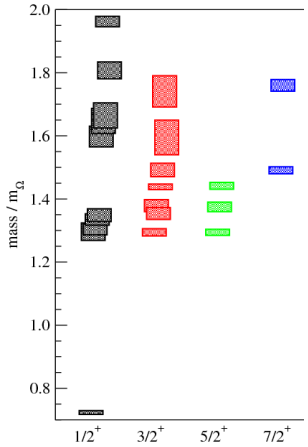

Extract

- Extract information from measured observables

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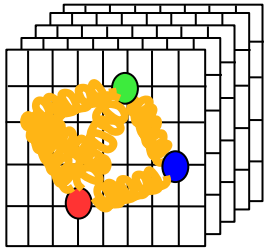
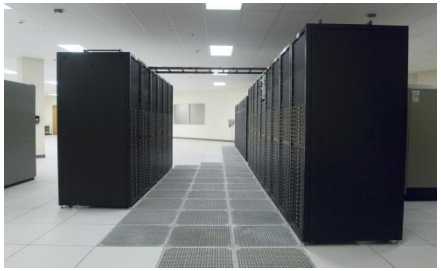


Few big jobs
Few big files



Analyze

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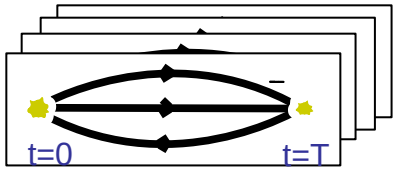

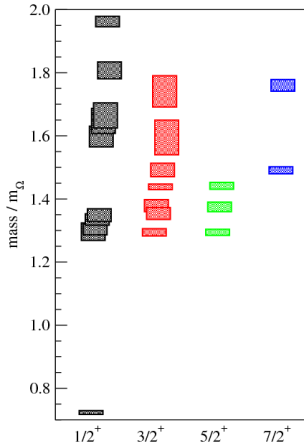

Extract

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Many small jobs
Many big files

I/O movement

Computational Requirements

Gauge generation : Analysis

Current calculations

- Weak matrix elements: 1 : 1
- Baryon spectroscopy: 1 : 10
- Nuclear structure: 1 : 4

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10	:	1	(2005)
1	:	4	(2011)

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Computational Requirements:

Gauge Generation	:	Analysis	
10	:	1	(2005)
1	:	4	(2011)

Core work: Dirac inverters - use GPU-s

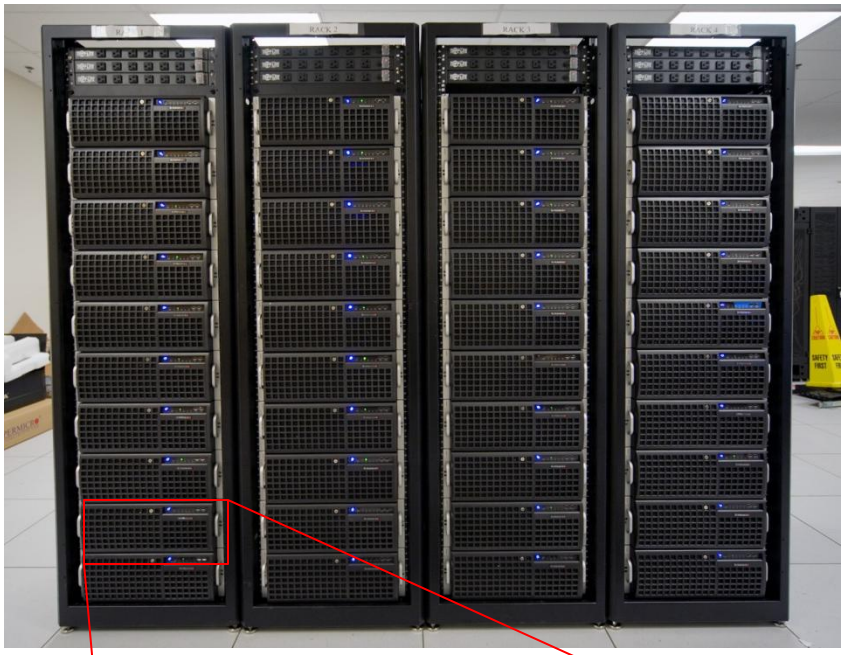
SciDAC Impact

- Software development
  - QCD friendly API's and libraries: enables high user productivity
  - Allows rapid prototyping & optimization
  - Significant software effort for GPU-s

- Algorithm improvements
  - Operators & contractions: clusters (Distillation: PRL (2009))
  - Mixed-precision Dirac-solvers: INCITE+clusters+GPU-s, 2-3X
  - Adaptive multi-grid solvers: clusters, ~8X (?)

- Hardware development via USQCD Facilities
  - Adding support for new hardware
  - GPU-s

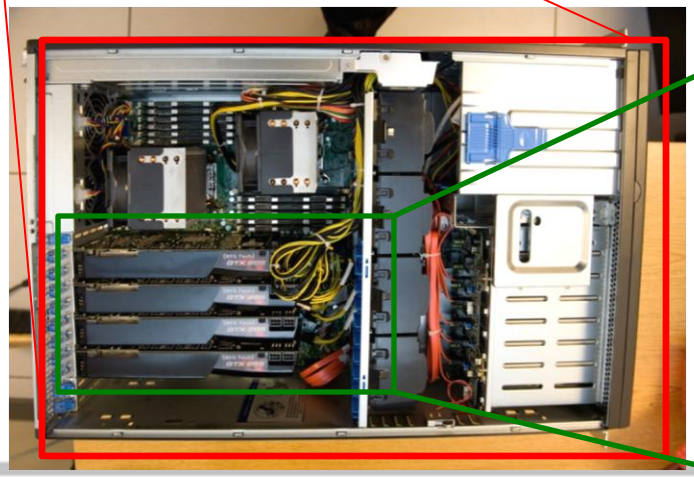
Hardware: ARRA GPU Clusters

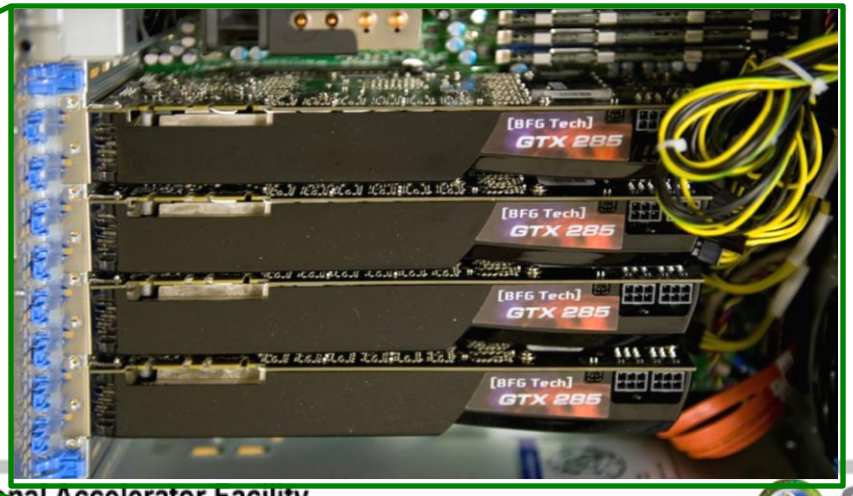


GPU clusters: ~530 cards

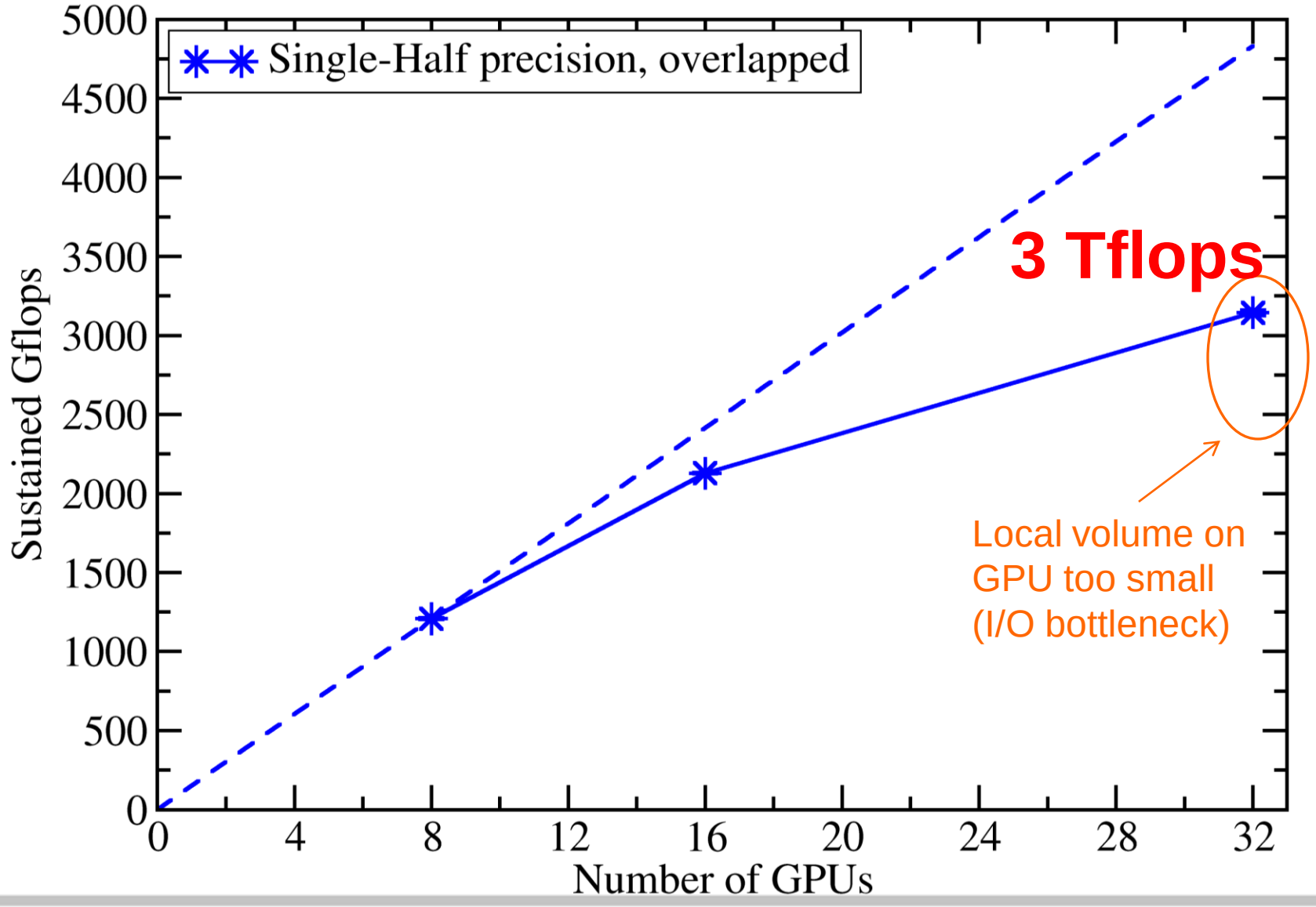
Quads
- 2.4 GHz Nehalem
- 48 GB memory / node
- 117 nodes x 4 GPUs -> 468 GPUs

Singles
- 2.4 GHz Nehalem
- 24 GB memory / node
- 64 nodes x 1 GPU -> 64 GPUs



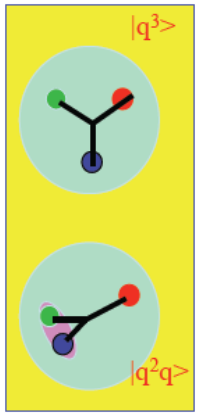


Inverter Strong Scaling: $V=32^3 \times 256$



Where are the "Missing" Baryon Resonances?

- What are collective modes?
- Is there "freezing" of degrees of freedom?
- What is the structure of the states?



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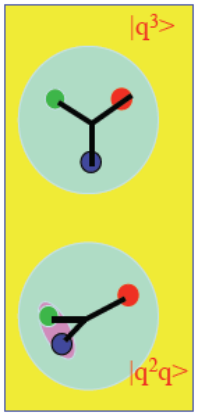
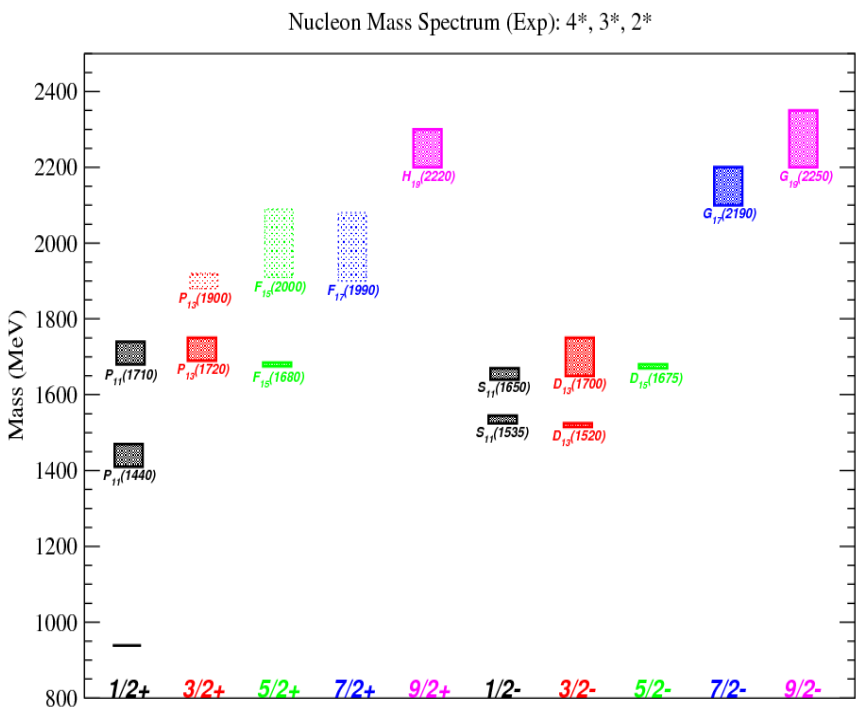
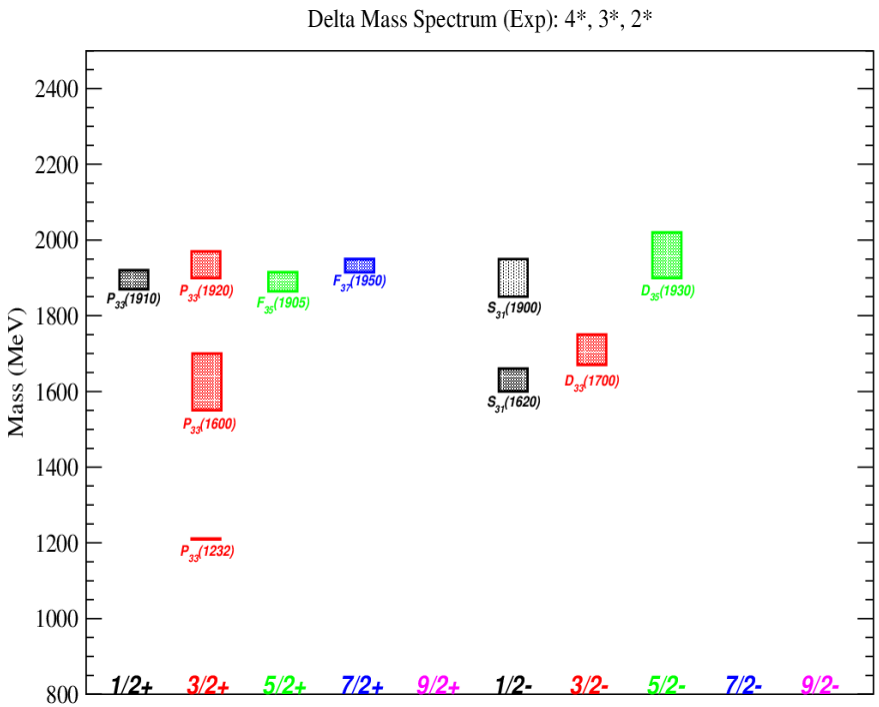


Nucleon & Delta spectrum
PDG uncertainty on
B-W mass





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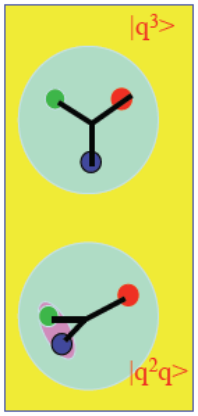

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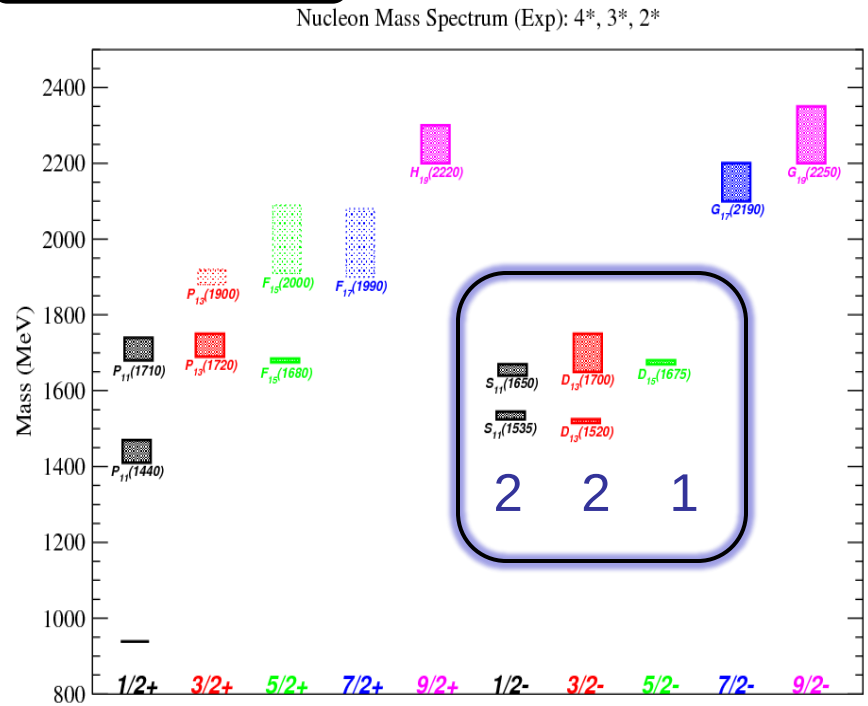
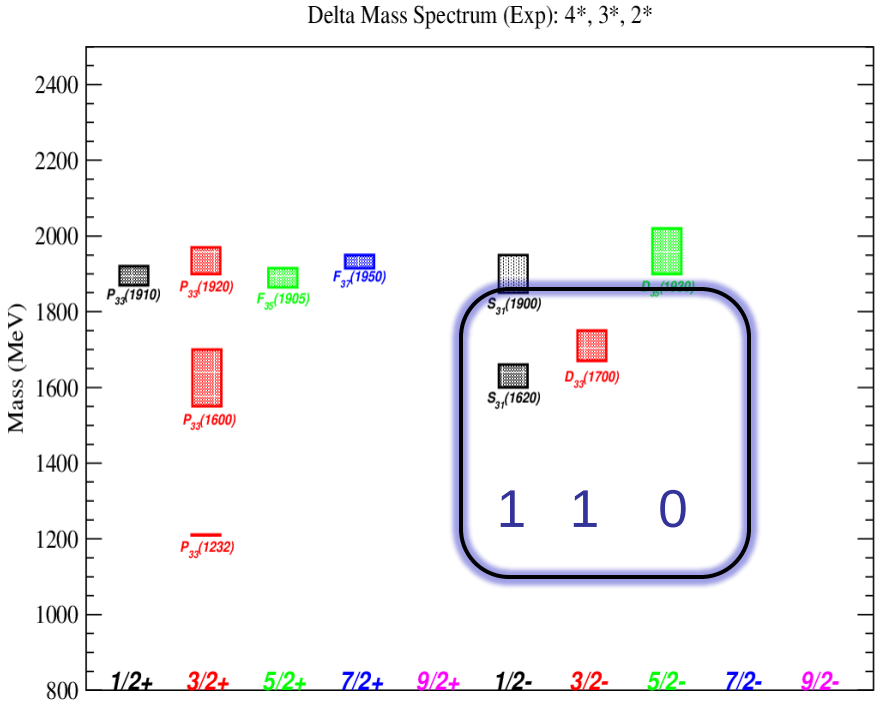
QM predictions





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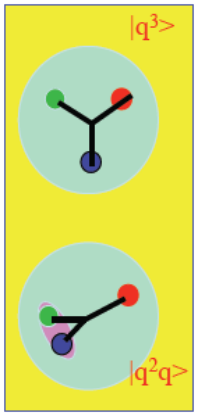

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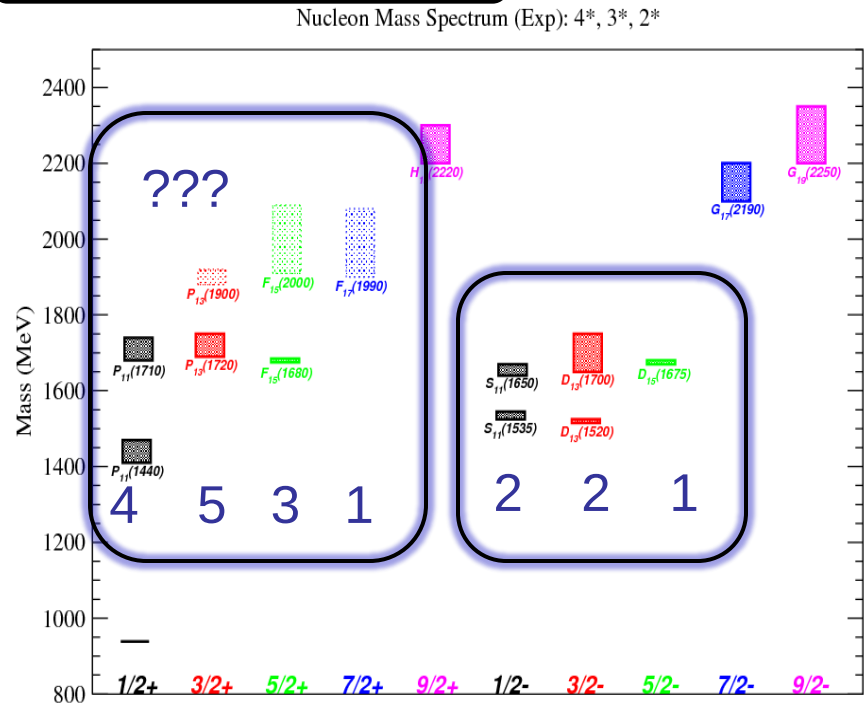
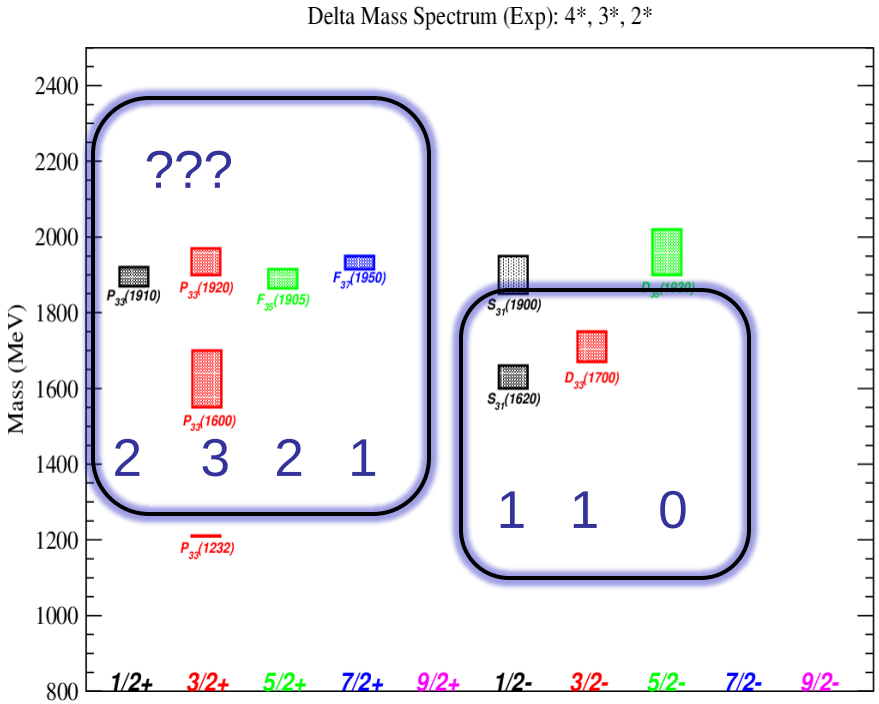
Quark Model predictions

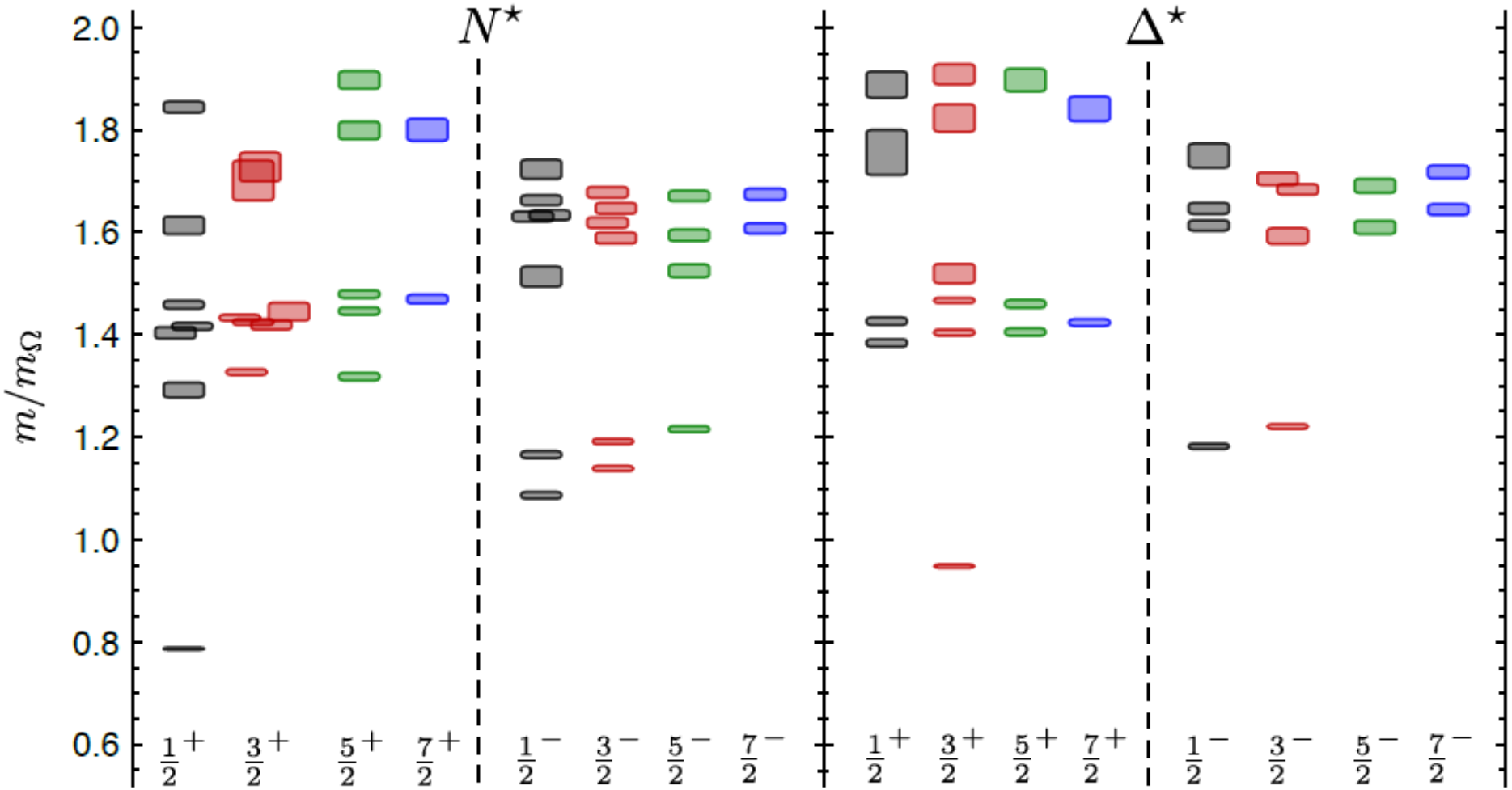




Spin identified Nucleon & Delta spectrum

arXiv:1104.5152

$m_\pi \sim 520$MeV



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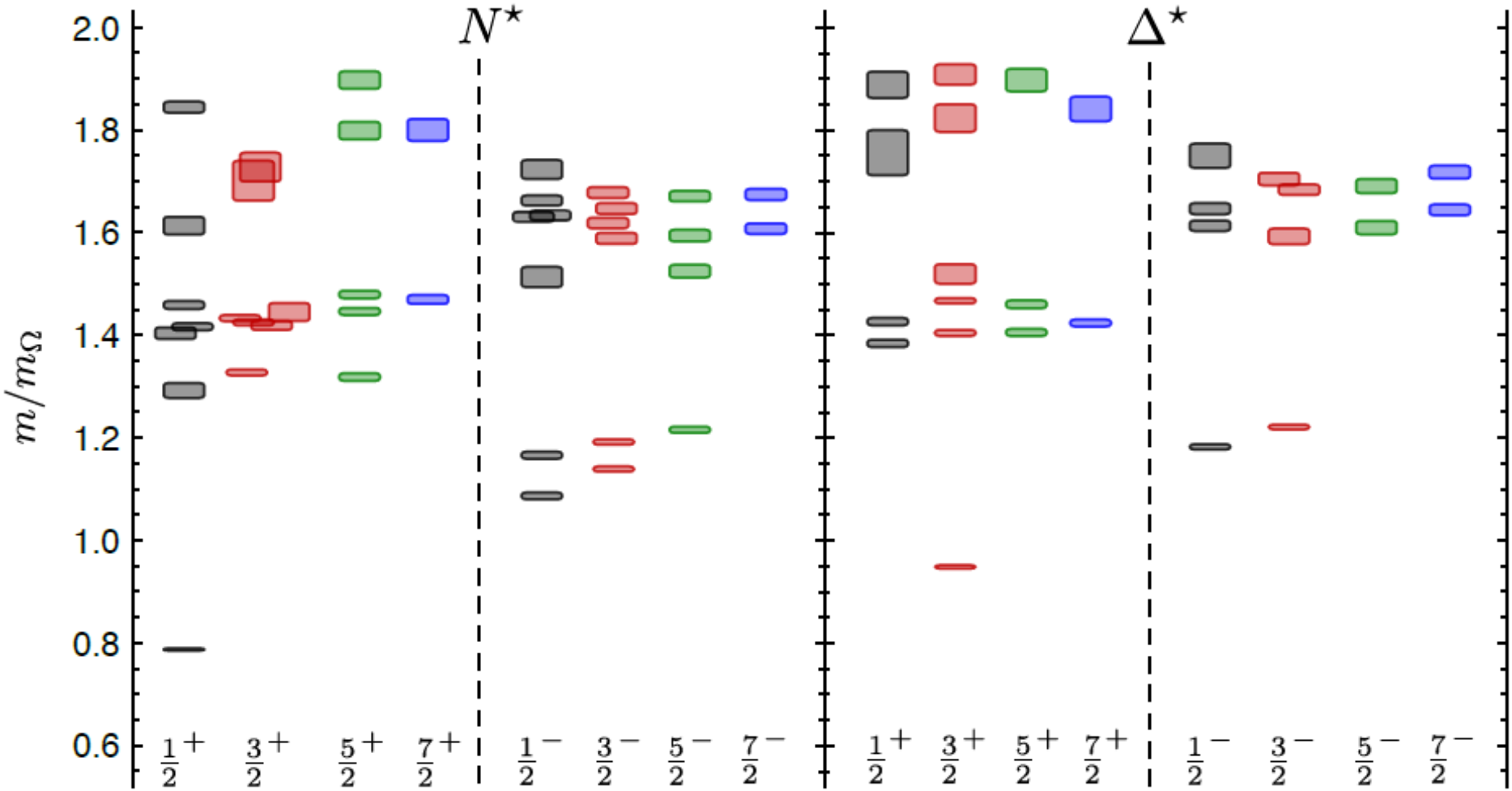

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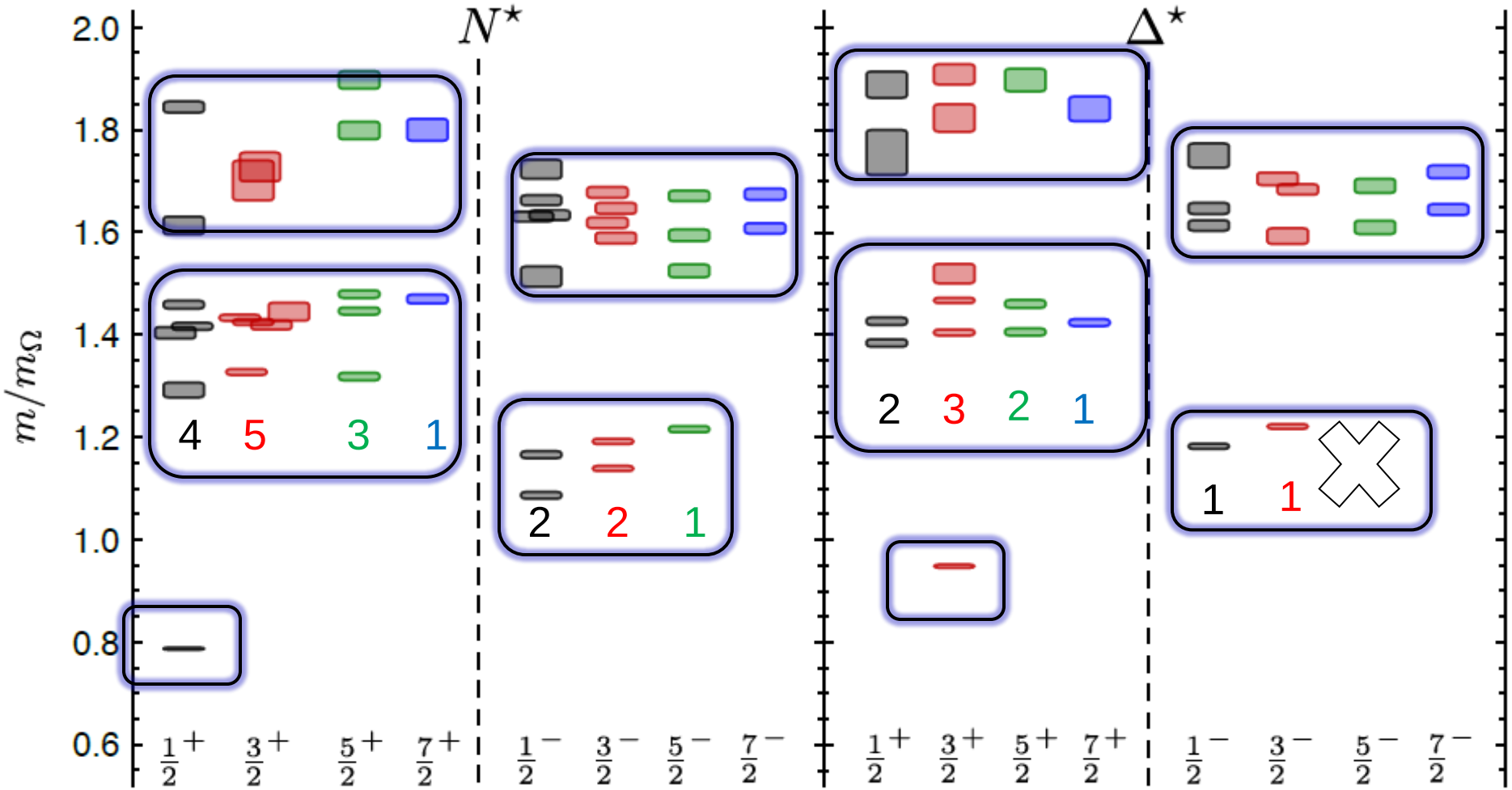

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Mass and overlaps: assign into multiplets

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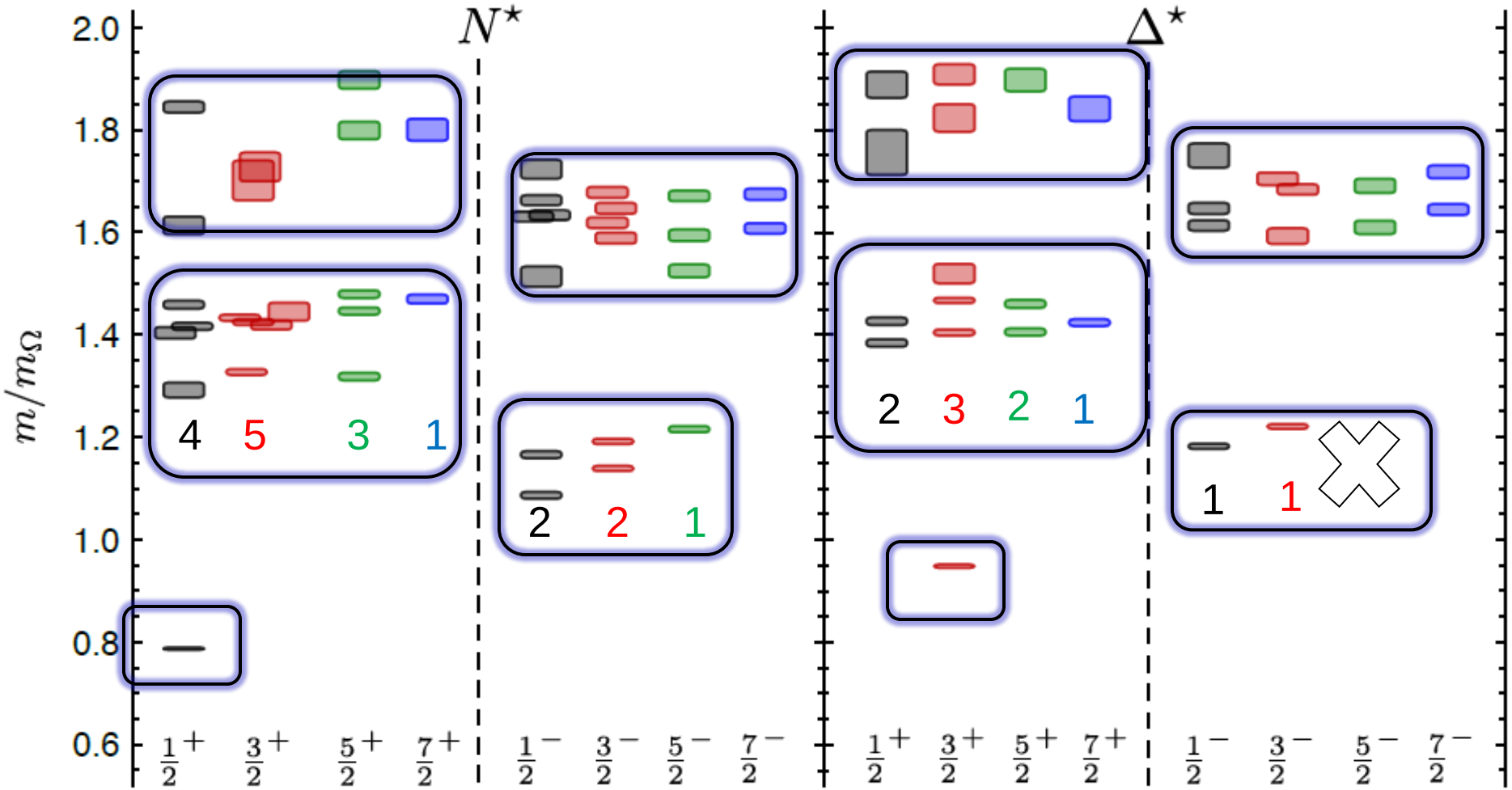

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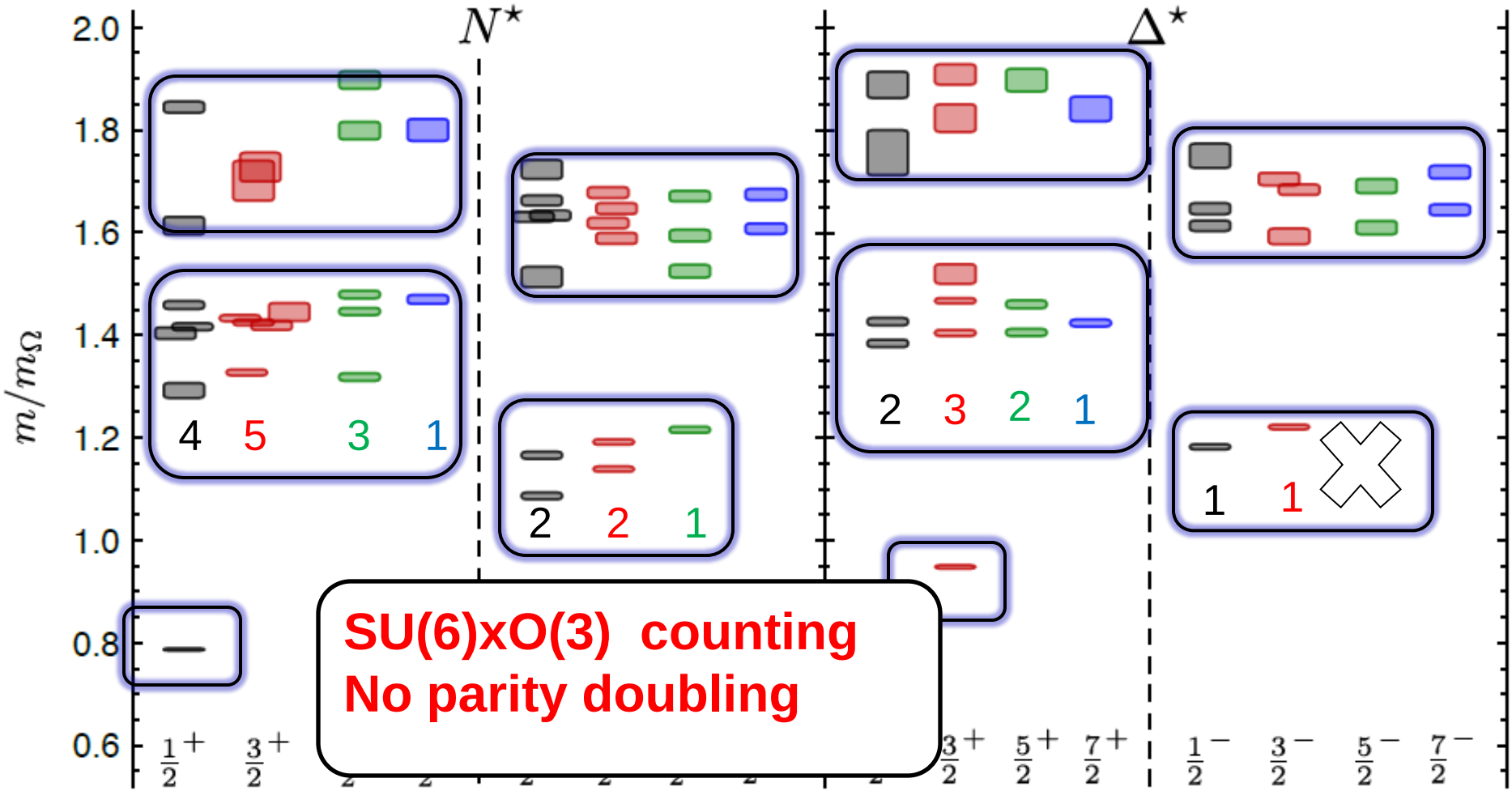
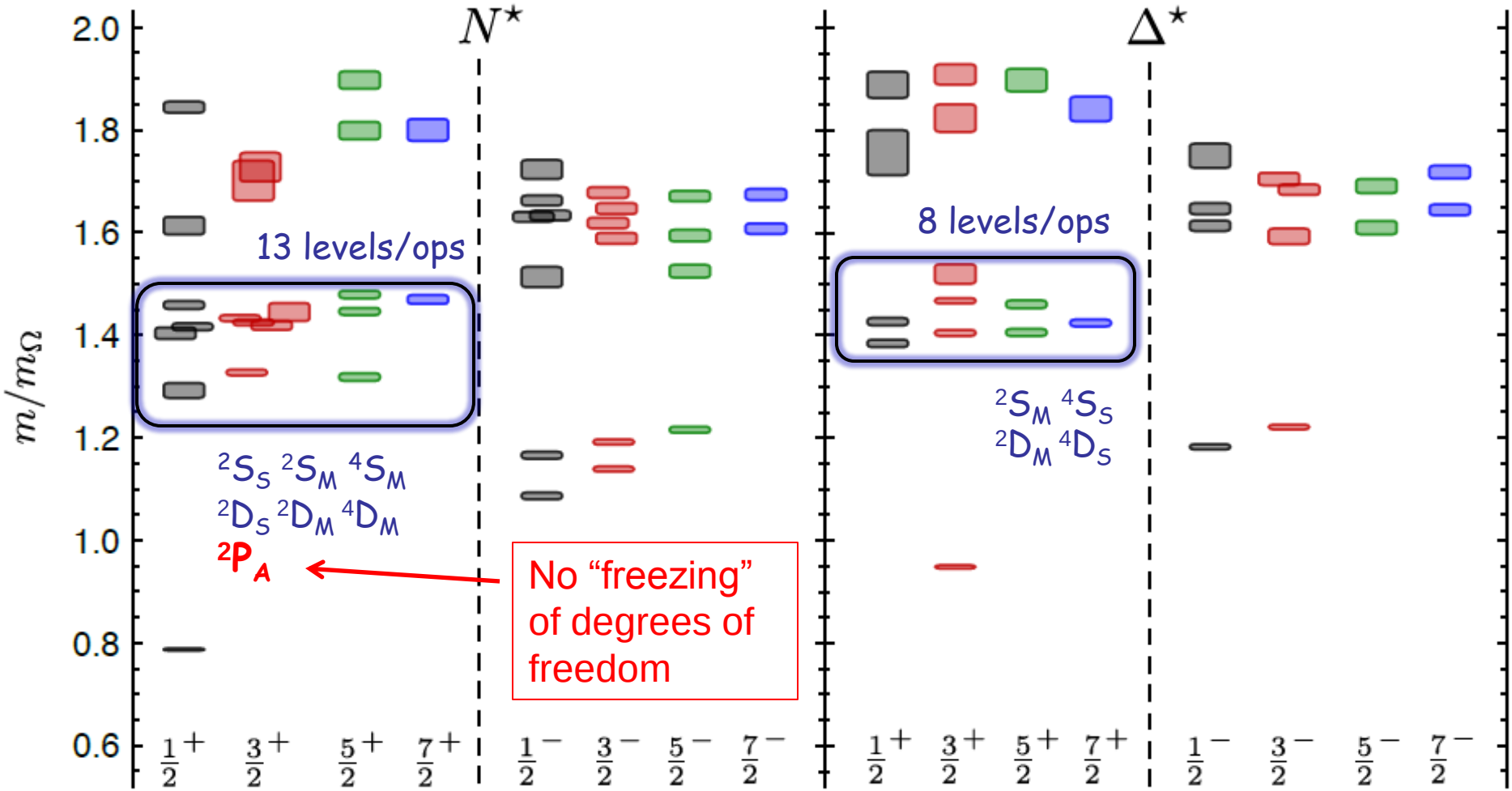


SU(6)xO(3) counting
No parity doubling

N=2 J^+ Nucleon & Delta spectrum

Discern structure: spectral overlaps

Significant mixing in J^+



Summary & prospects

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Results for baryon excited state spectrum:

- No “freezing” of degrees of freedom nor parity doubling
- Broadly consistent with non-relativistic quark model
- Add multi-particles $\rightarrow$ baryon spectrum becomes denser

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Results for baryon excited state spectrum:

- No "freezing" of degrees of freedom nor parity doubling
- Broadly consistent with non-relativistic quark model
- Add multi-particles $\rightarrow$ baryon spectrum becomes denser

Short-term plans: resonance determination!

- Lighter pion masses (230MeV available)
- Extract couplings in multi-channel systems (with π, η, K…)

Next 3-5 years

Need SciDAC-3 and partnerships

Current/future activities:

- USQCD researchers: co-designers BG/Q - improved cache usage
- Collaboration w/ Intel Parallel Computing Labs – improving codes
- Development of QUDA GPU software codes: hugely successful
- Exploiting domain decomposition techniques:
  - Push into integrators
  - Multigrid based inverters
- Improving physics-level algorithms/software:
  - Measurement methods for spectroscopy, hadron & nuclear structure

Developing for Exascale

Backup slides

- The end