Hadron Spectroscopy from QCD

Robert Edwards
Jefferson Lab

NERSC 2014

Hadron spectroscopy

- Determination of hadron spectrum of QCD a central goal in NP
- Several experiments worldwide

LHCb

ATLAS CMS

CLAS12 GlueX

+ others at 12 GeV JLab

BESIII KLOE2

COMPASS

panda

+ others at GSI

Belle II

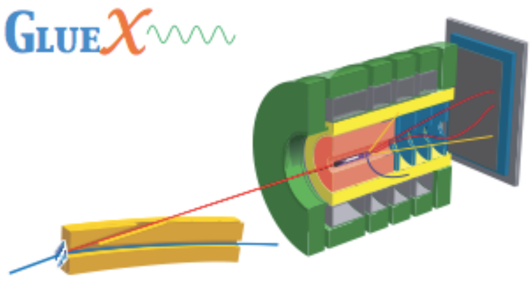
ELSA MAMI J-PARC Spring-8

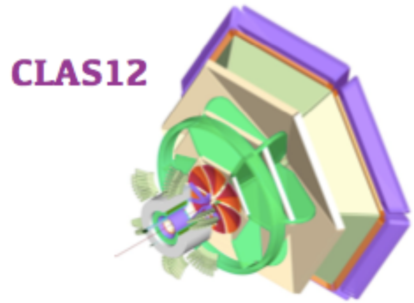
Hadron spectroscopy

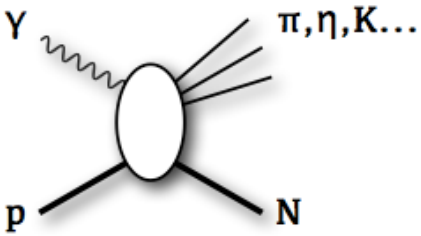
- Determination of hadron spectrum of QCD a central goal in NP
- Several experiments worldwide

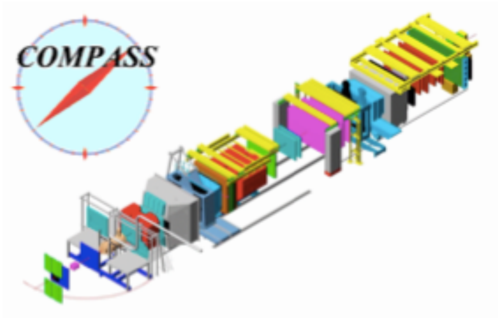
- Our project intends to compute the spectrum of QCD to inform and guide the experimental programs

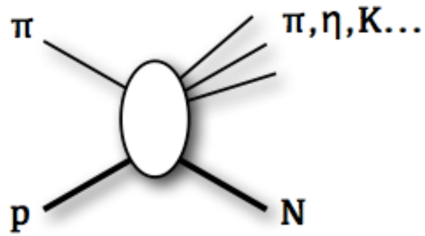
Spectrum – light meson experiments

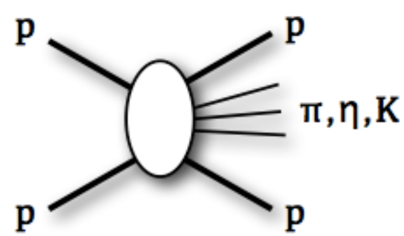


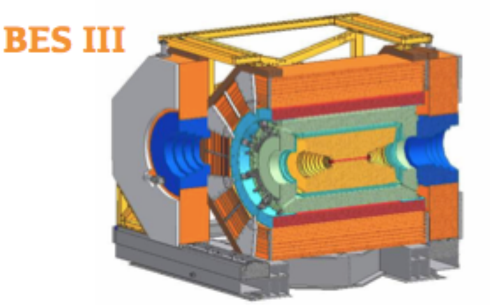


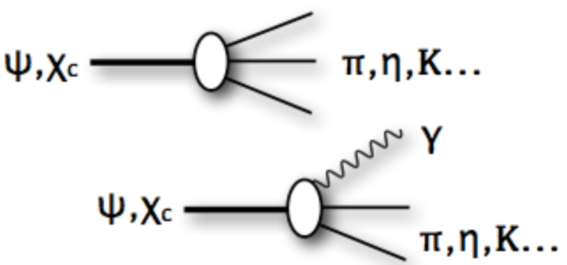






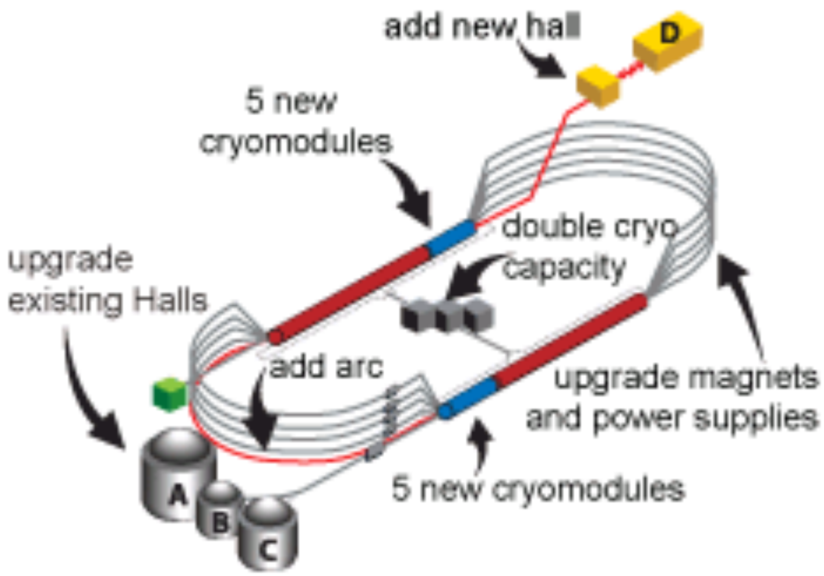






Nuclear Physics & Jefferson Lab

JLab undergoing a $310M major upgrade



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

NSAC milestones circa 2008

Table 4: Milestone Progress in Hadronic Physics

Year	Milestone	Complete?	Status Assessment
2009 HP3	Complete the combined analysis of available data on single π, η, and K photo-production of nucleon resonances and incorporate the analysis of two-pion final states into the coupled-channel analysis of resonances.	No	Expect to Not Achieve Fully
2014 HP9	Perform lattice calculations in full QCD of nucleon form factors, low moments of nucleon structure functions and low moments of generalized parton distributions including flavor and spin dependence.	No	Expect to Exceed
2014 HP10	Carry out ab initio microscopic studies of the structure and dynamics of light nuclei based on two-nucleon and many-nucleon forces and lattice QCD calculations of hadron interaction mechanisms relevant to the origin of the nucleon-nucleon interaction.	No	Expect to Achieve

Spectrum

Structure

Interactions

2018	HP15 (new)	The first results on the search for exotic mesons using photon beams will be completed.
2015	FI12 (new)	Analyze the implications, for possible new fundamental interactions, of precise measurements of parity-violating electron scattering asymmetries, weak decays of nuclei, light hadrons and leptons, and the muon g-factor.
2020	FI15 (new)	Obtain initial results from an experiment to extend the limit on the electric dipole moment of the neutron by two orders of magnitude

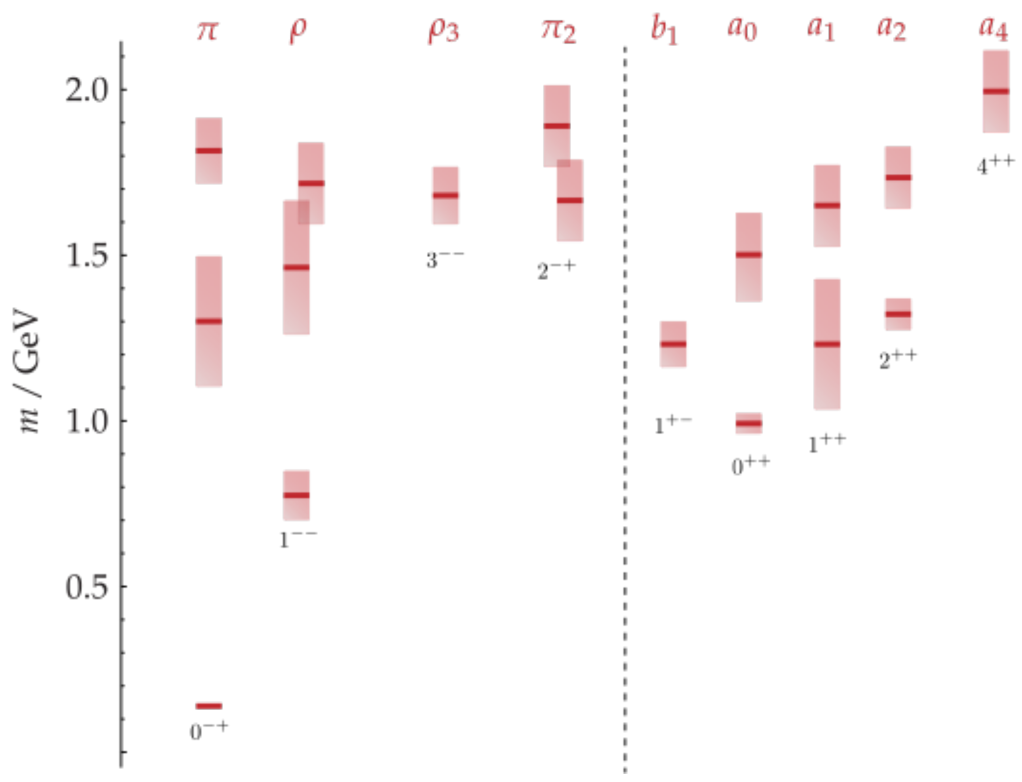
Spectrum

Fundamental symmetries

Experimental meson spectrum

- Mesons classified by their conserved quantum numbers
  - Spin, isospin, charge-conjugation J^{PC}

ISOSPIN=1 MESON SPECTRUM



Experimental meson spectrum

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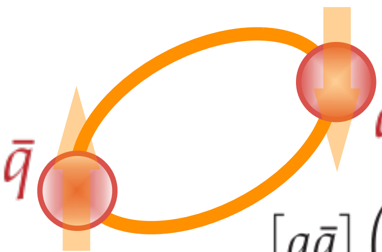
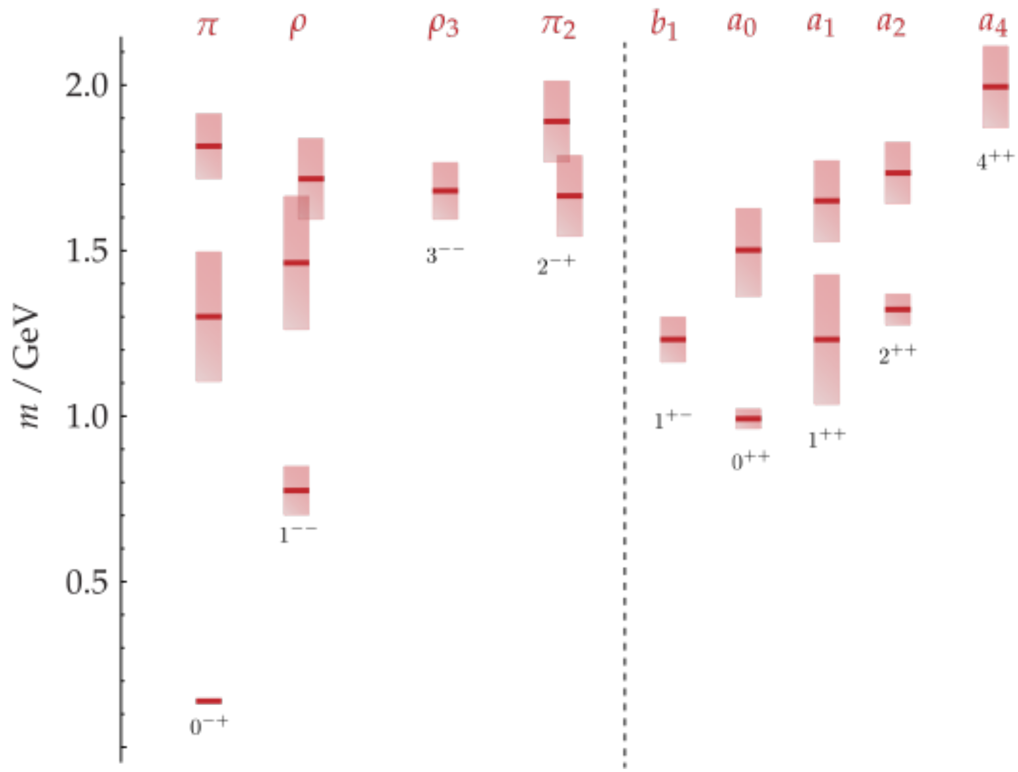


$$[q\bar{q}]\left(n\,^{2S+1}L_J\right)$$

$$L = 0 \;:\; 0^{-+}, 1^{--}$$
$$L = 1 \;:\; 1^{+-},\, (0,1,2)^{++}$$
$$L = 2 \;:\; 2^{-+},\, (1,2,3)^{--}$$
$$\vdots$$

ISOSPIN=1 MESON SPECTRUM



Experimental meson spectrum

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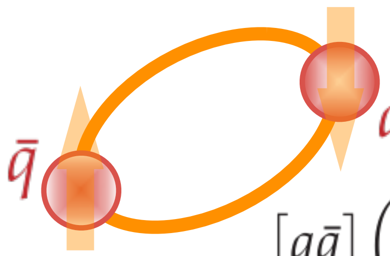

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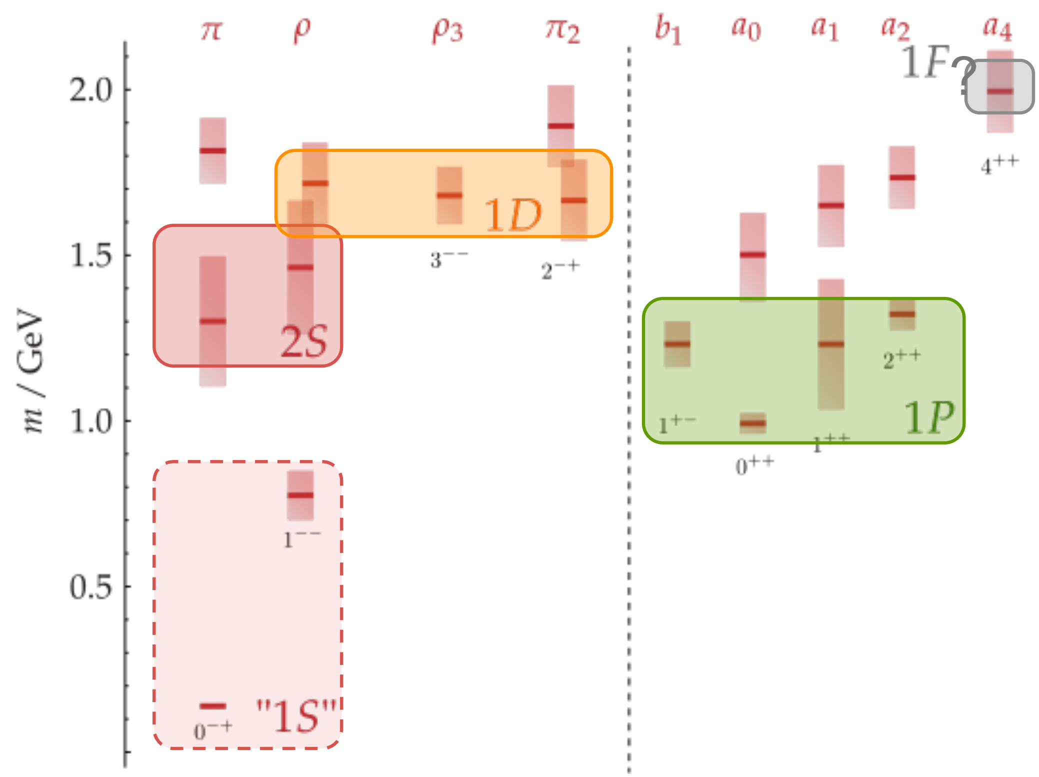
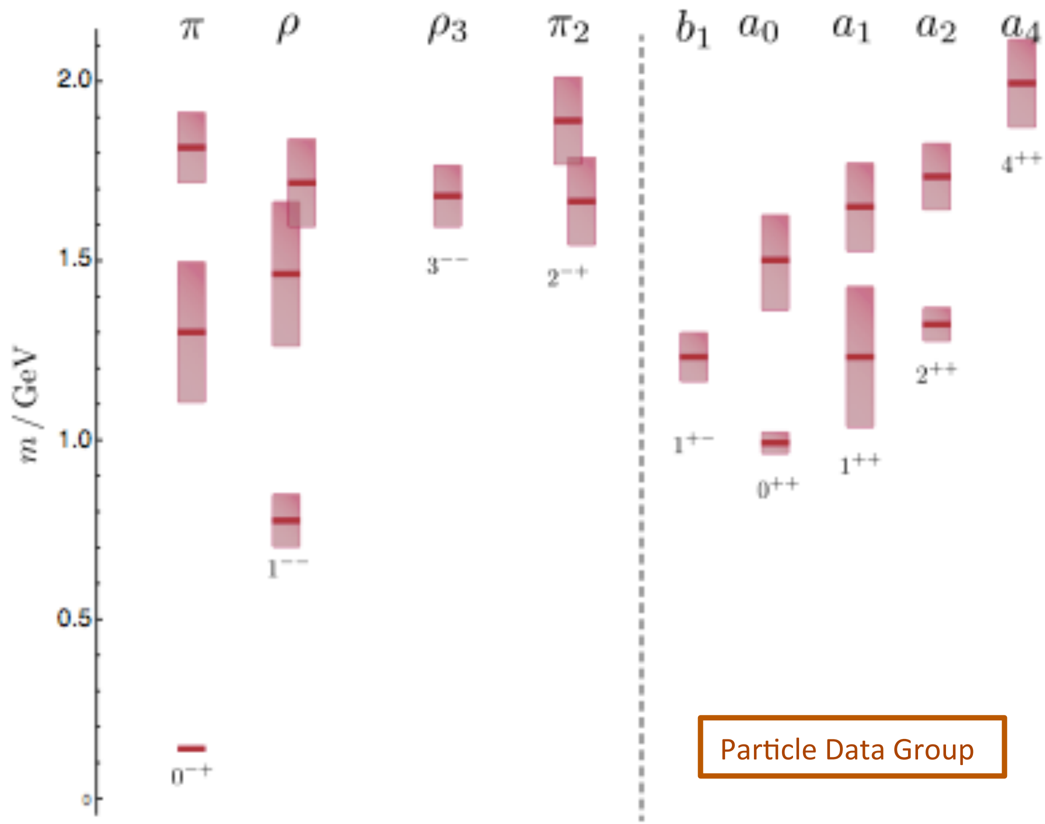


Exotic mesons

Quark-antiquark spatial (only) excitations exclude $\mathbf{J^{PC}}$ $\mathbf{0^{--}, 0^{+-}, 1^{-+}, 2^{+-}}$

"Smoking gun signature"



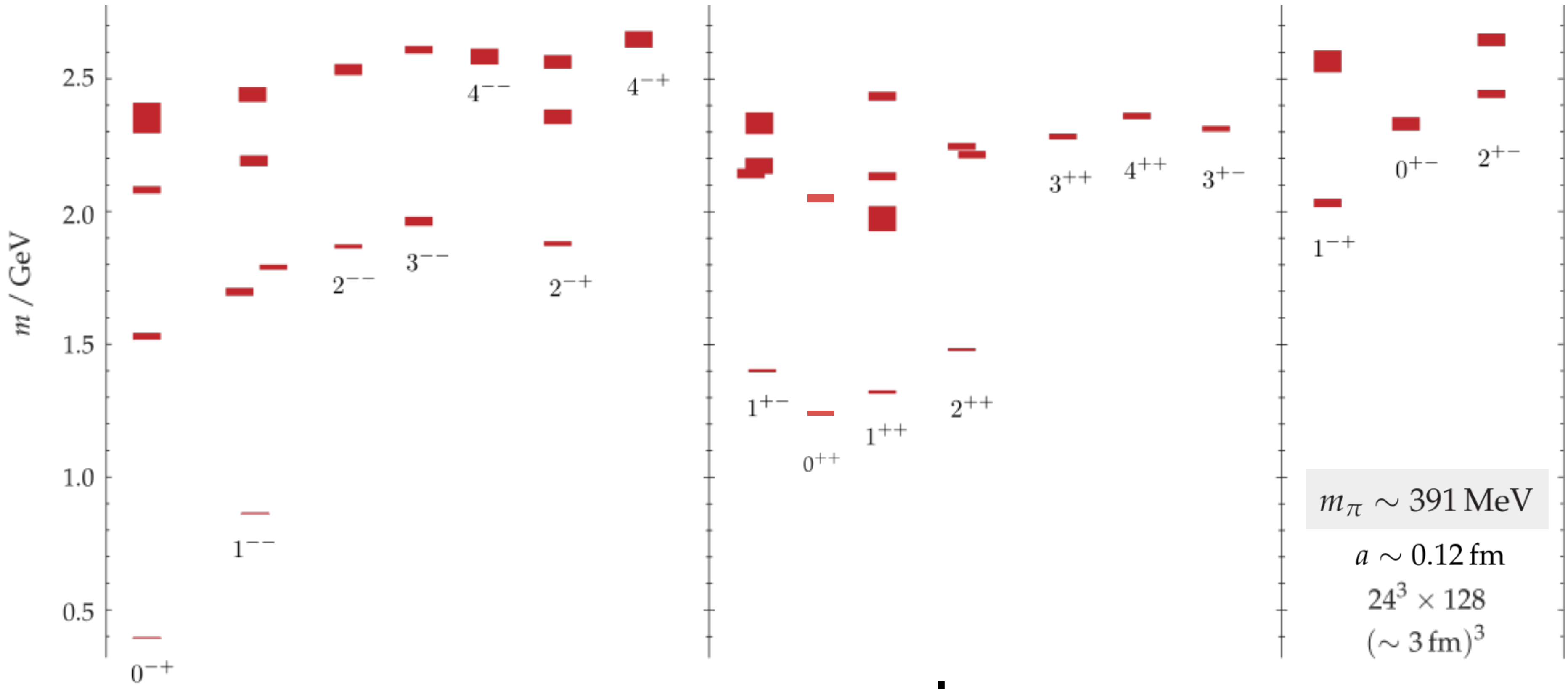
Possible explanation: "hybrid" mesons $q\bar{q}\, G_{\mathbf{8_c}}$

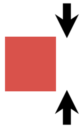
Many models, many different/conflicting predictions

Need theoretical guidance from QCD

Meson spectrum

- A Lattice QCD determination of the meson spectrum

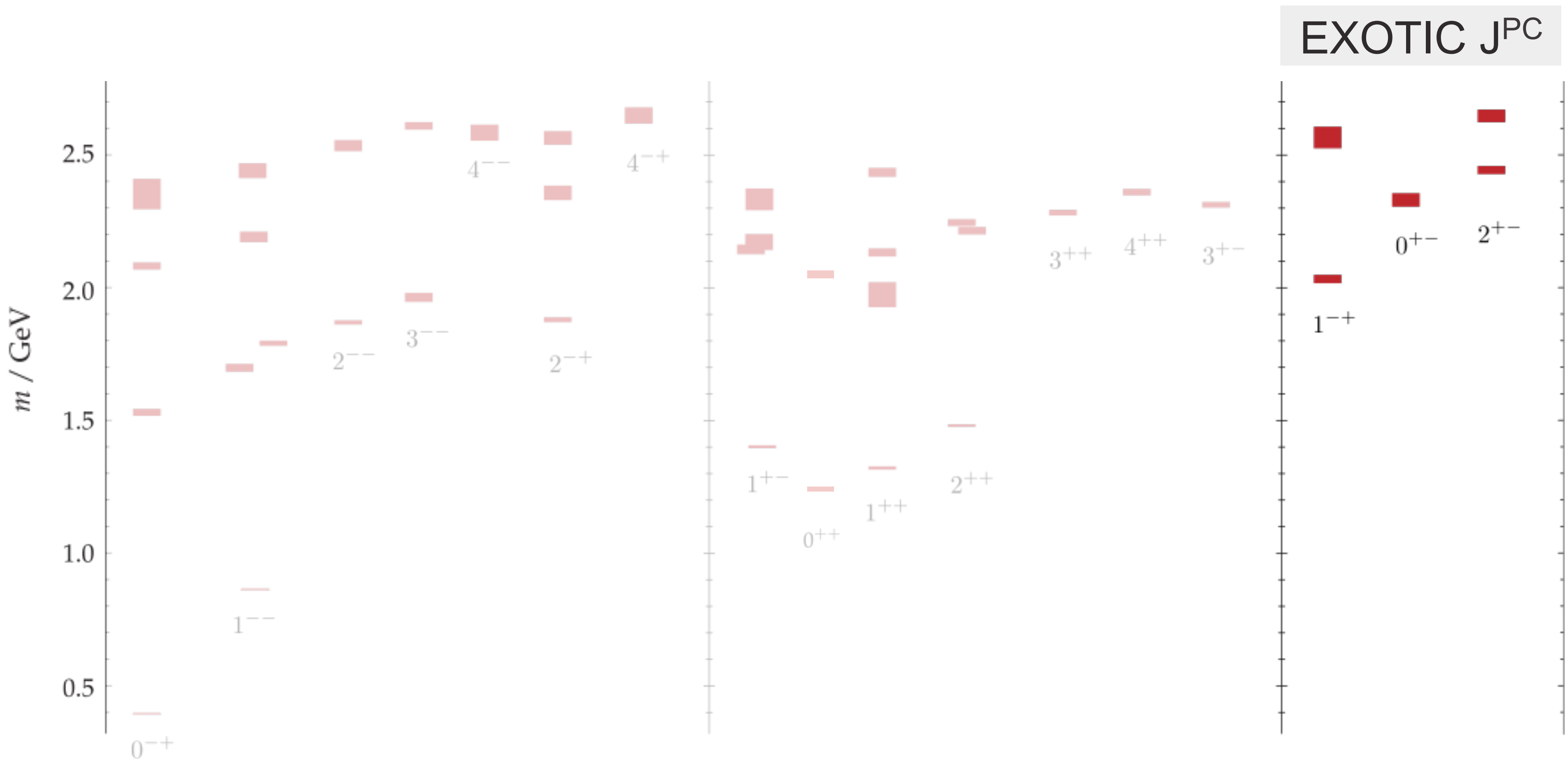




arXiv:1004.4930, 1309.2608

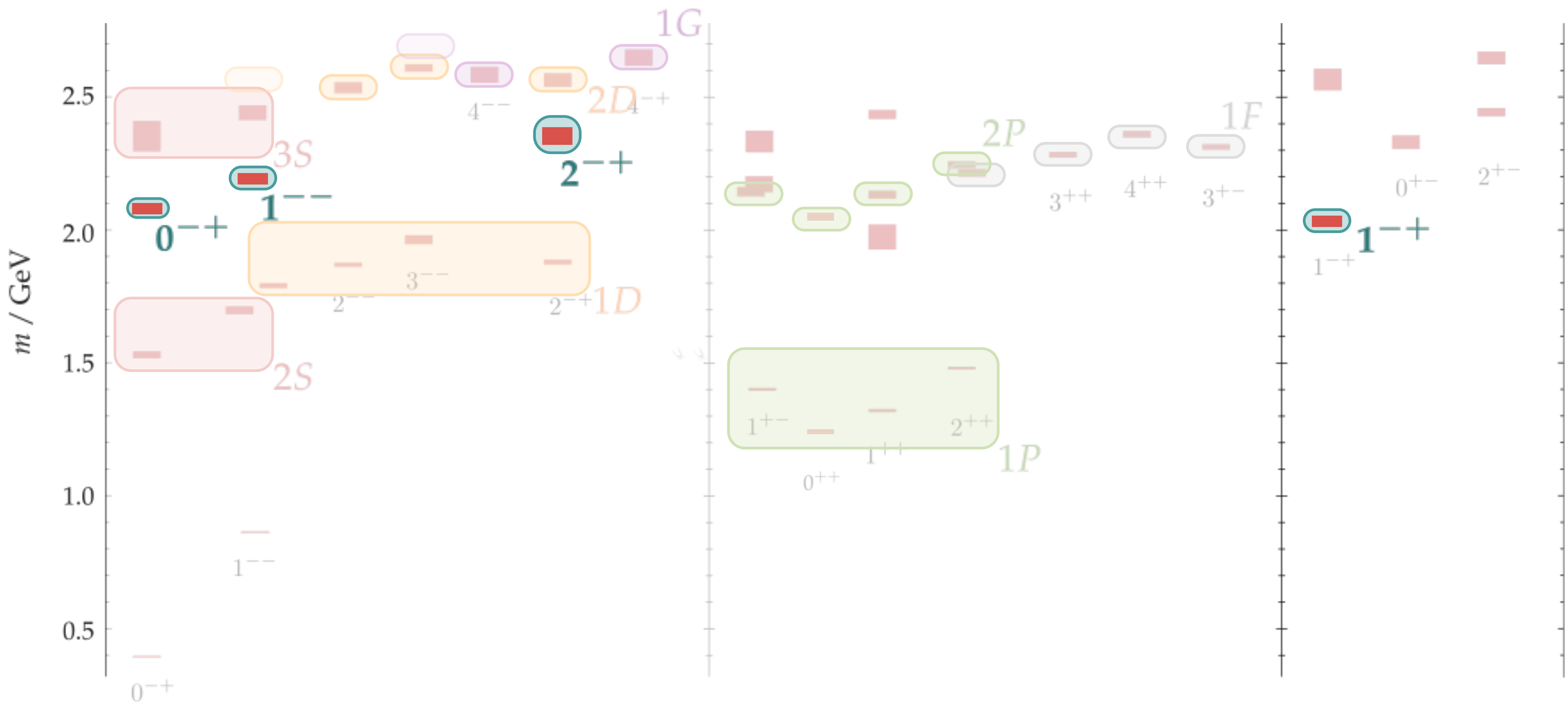
Meson spectrum

- **Exotic J^{PC}** states are present



Meson spectrum

- “super”-multiplet of hybrid mesons roughly 1.3 GeV above the ρ



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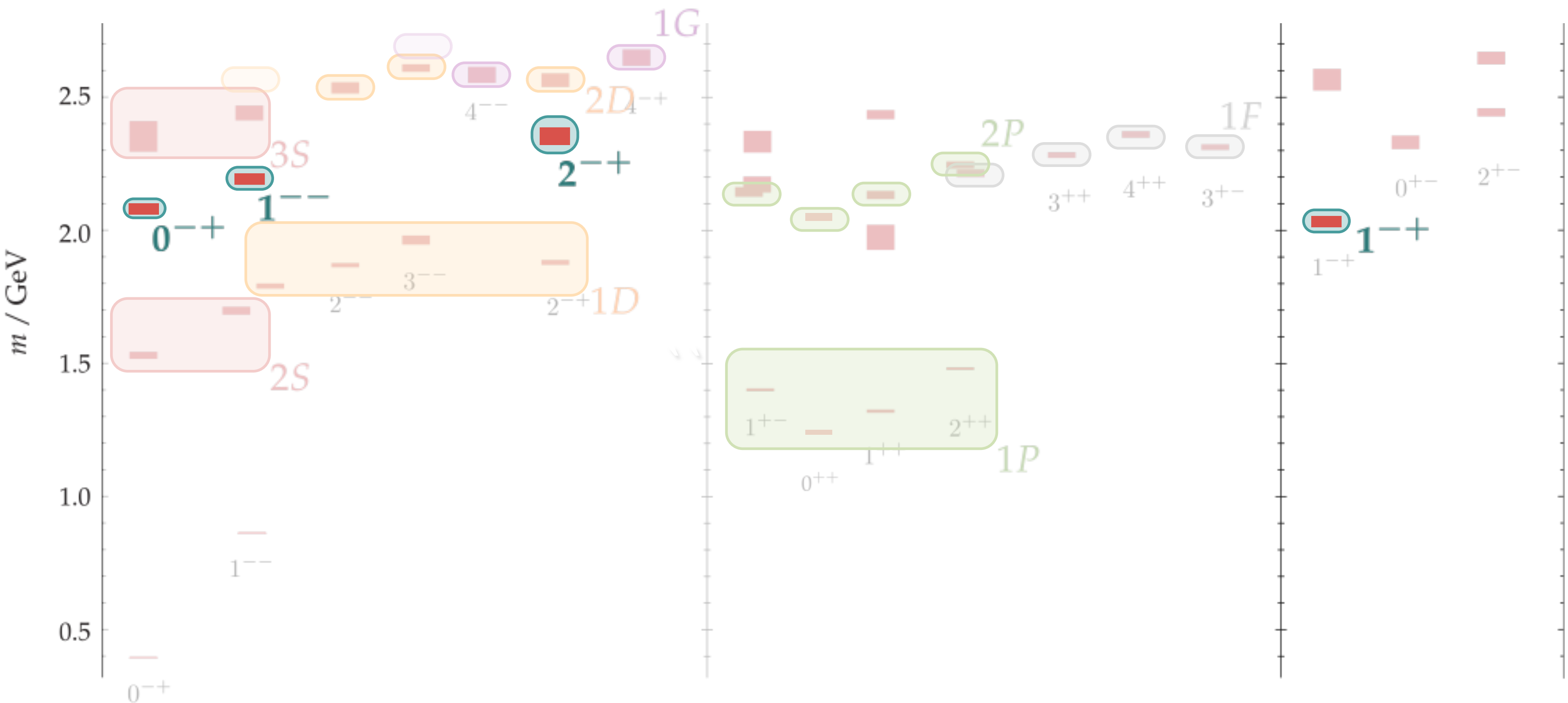
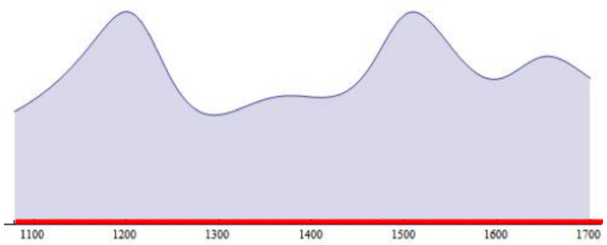
New scale in QCD

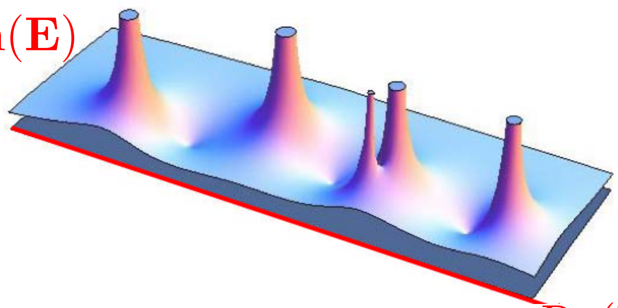


- Are we done? No, need decays!

Resonances

- Most hadrons are resonances
  - E.g., πN ➔πN



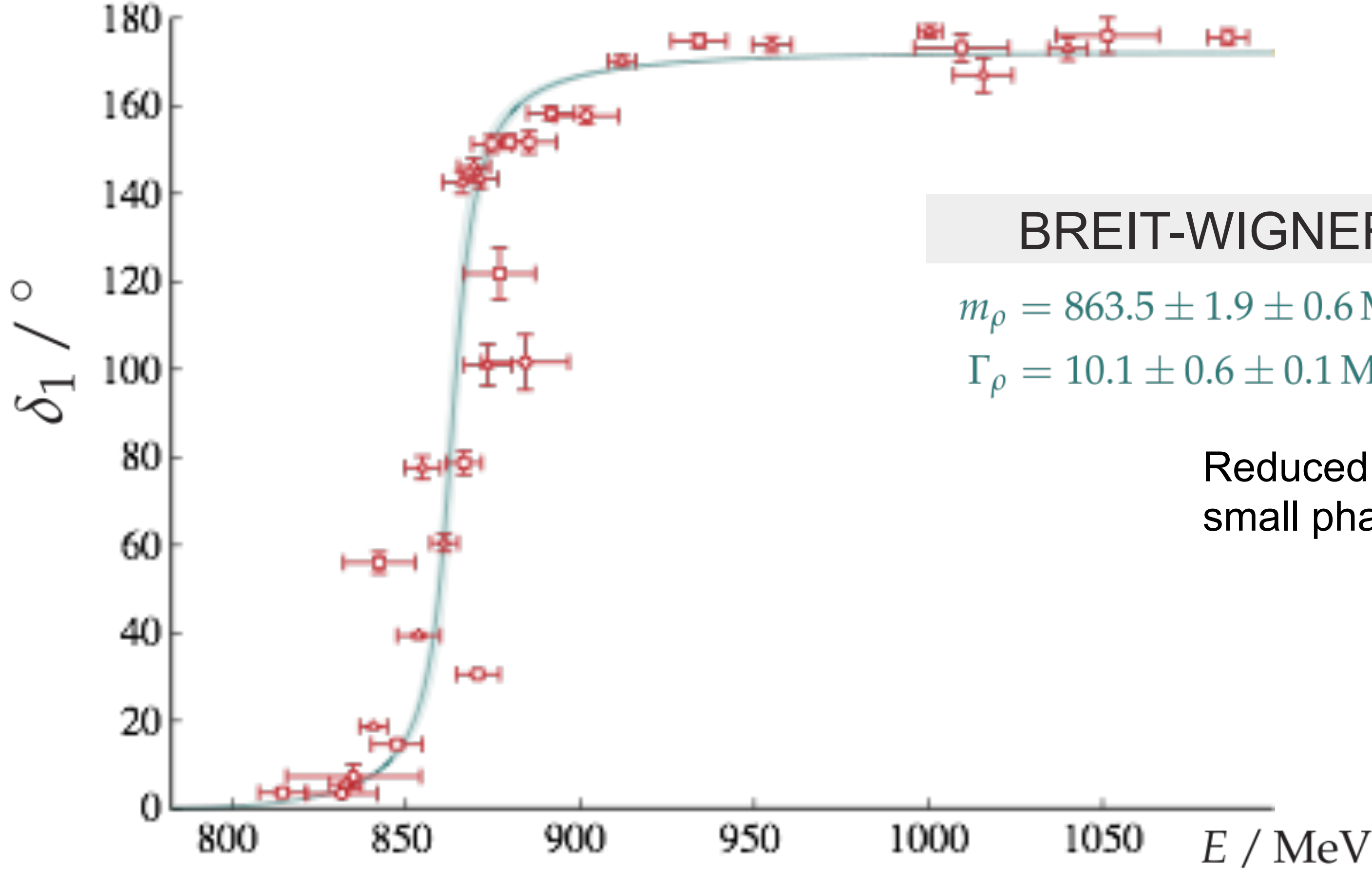


  - Formally defined as a pole in scattering amplitude
  - Different channels should have same pole location
  - Pole structure gives decay information

- Can we predict hadron properties from first principles? Yes

Isospin=1 ($J^{PC}=1^{--}$) ππ scattering

- Breit-Wigner fit to the energy dependence



BREIT-WIGNER

$$m_\rho = 863.5 \pm 1.9 \pm 0.6\,\mathrm{MeV}$$

$$\Gamma_\rho = 10.1 \pm 0.6 \pm 0.1\,\mathrm{MeV}$$

Reduced width from small phase-space

ORNL resources

$$g_{\rho\pi\pi} = 4.83 \pm 0.13 \pm 0.02$$

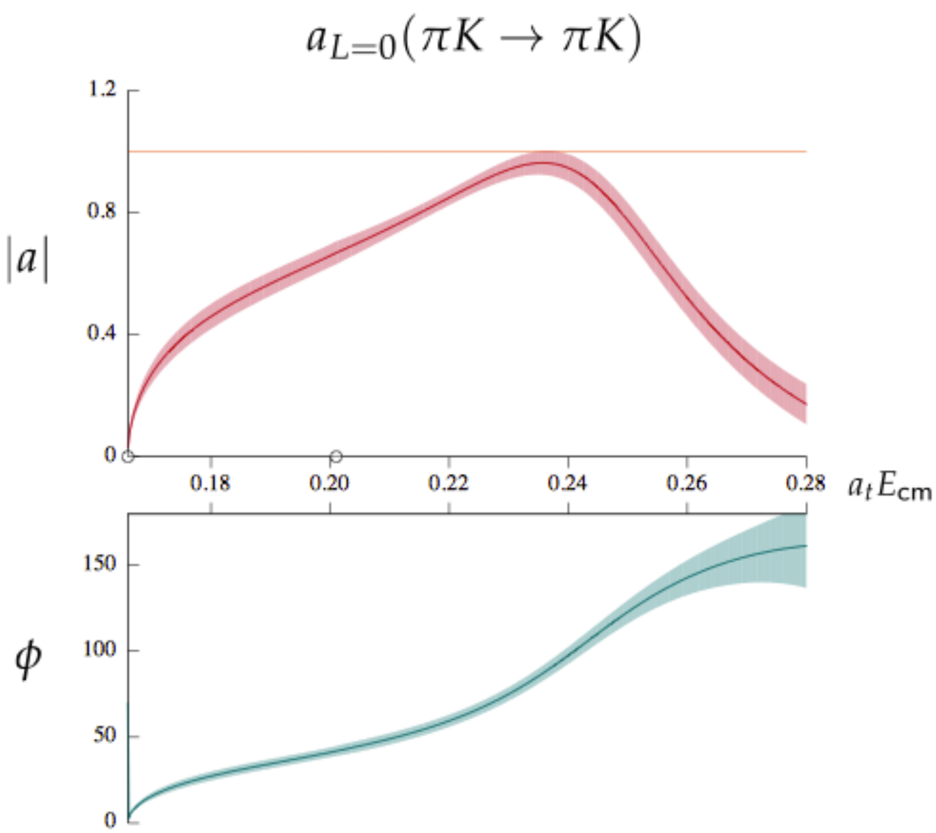
arxiv:1212.0830

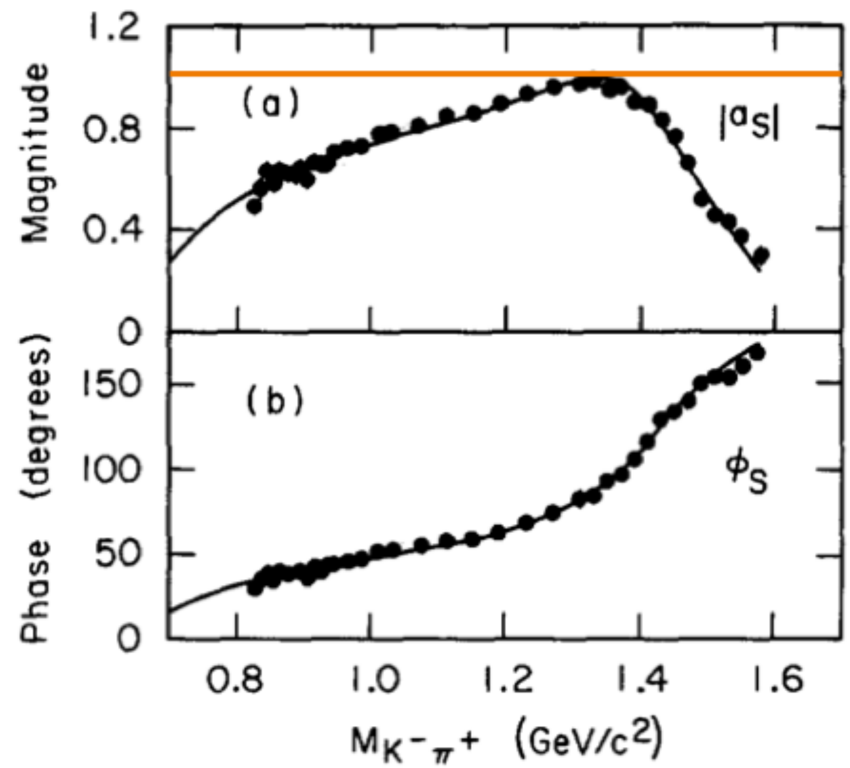
$$m_\pi \sim 391\,\mathrm{MeV}$$

More complicated example: Kπ/Kη

$J^P = 0^+$

First LQCD determination of a scalar resonance





LASS, NPB296 493

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Impact on experiment

arxiv:1208.1244

Physics Opportunities with the 12 GeV Upgrade at Jefferson Lab

Jozef Dudek, Rolf Ent, Rouven Essig, Krishna Kumar, Curtis Meyer, Robert McKeown, Zein Eddine Meziani, Gerald A. Miller, Michael Pennington, David Richards, Larry Weinstein, Glenn Young

arxiv:1210.4508 & approved JLab proposal - second phase of GlueX project

PR12-13-003

An initial study of mesons and baryons containing strange quarks with GlueX

(A proposal to the 40th Jefferson Lab Program Advisory Committee)

A. AlekSejevs,[1] S. Barkanova,[1] M. Dugger,[2] B. Ritchie,[2] I. Senderovich,[2] E. Anassontzis,[3] P. Ioannou,[3] C. Kourkoumeli,[3] G. Voulgaris,[3] N. Jarvis,[4] W. Levine,[4] P. Mattione,[4] W. McGinley,[4] C. A. Meyer,[4,*]

⋮

The primary motivation of the GlueX experiment is to search for and ultimately study the pattern of gluonic excitations in the meson spectrum produced in γp collisions. Recent lattice QCD calculations predict a rich spectrum of hybrid mesons that have both exotic and non-exotic J^{PC}, corresponding to $q\bar{q}$ states ($q = u$, d, or s) coupled with a gluonic field. A thorough study of the

Impact on experiment

arxiv:1212.4891 - science case for JLab Hall B expt.

Studies of Nucleon Resonance Structure in Exclusive Meson Electroproduction

I. G. Aznauryan,[1,2] A. Bashir,[3] V. M. Braun,[4] S. J. Brodsky,[5,6] V. D. Burkert,[2] L. Chang,[7,8] Ch. Chen,[7,9,10] B. El-Bennich,[11,12] I. C. Cloët,[7,13] P. L. Cole,[14] R. G. Edwards,[2] G. V. Fedotov,[15,16] M. M. Giannini,[17,18] R. W. Gothe,[15] F. Gross,[2,19] Huey-Wen Lin,[20] P. Kroll,[21,4] T.-S. H. Lee,[7] W. Melnitchouk,[2] V. I. Mokeev,[2,16] M. T. Peña,[22,23] G. Ramalho,[22] C. D. Roberts,[7,10] E. Santopinto,[18] G. F. de Teramond,[24] K. Tsushima,[13,25] and D. J. Wilson[7,26]

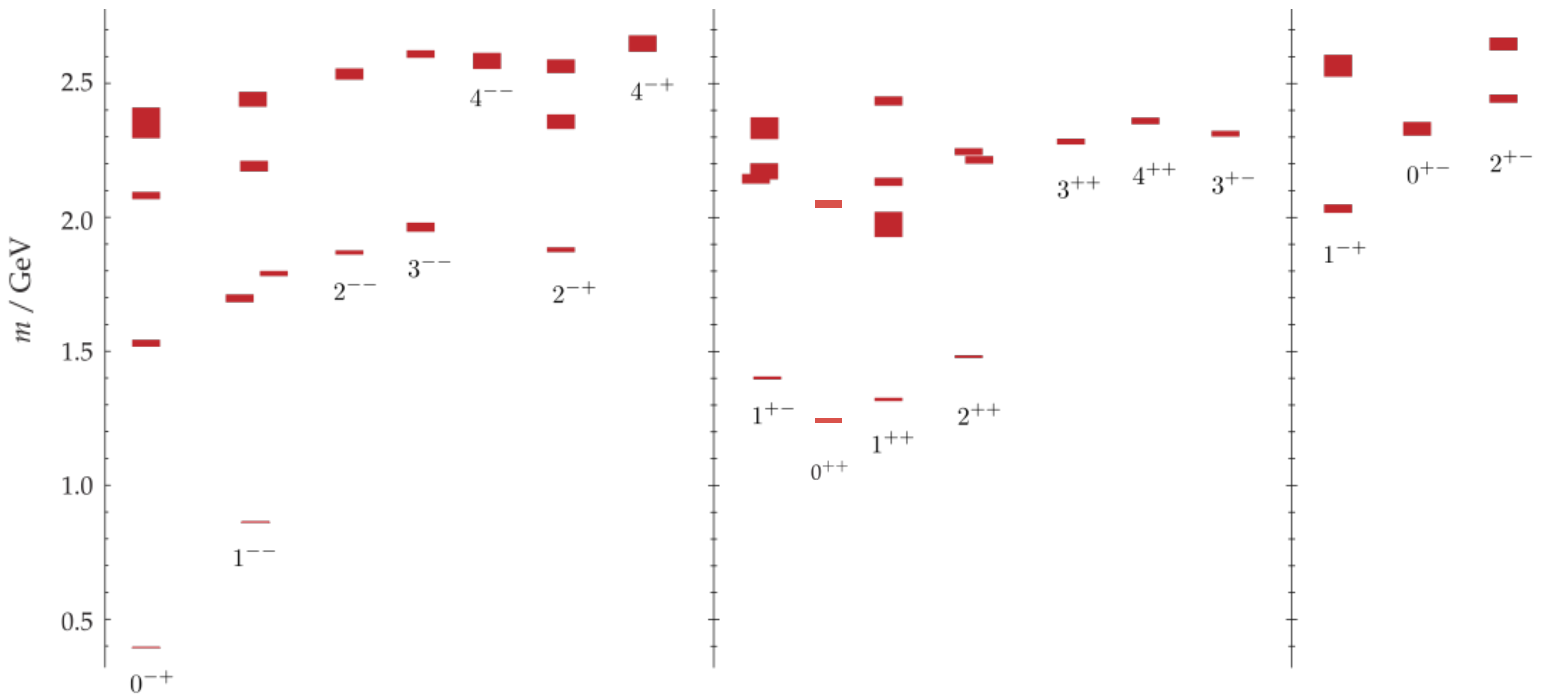
NSAC report – prominently features LQCD exotic meson spectroscopy supporting JLab

Report to the
Nuclear Science Advisory Committee
Implementing the 2007 Long Range Plan
January 31, 2013

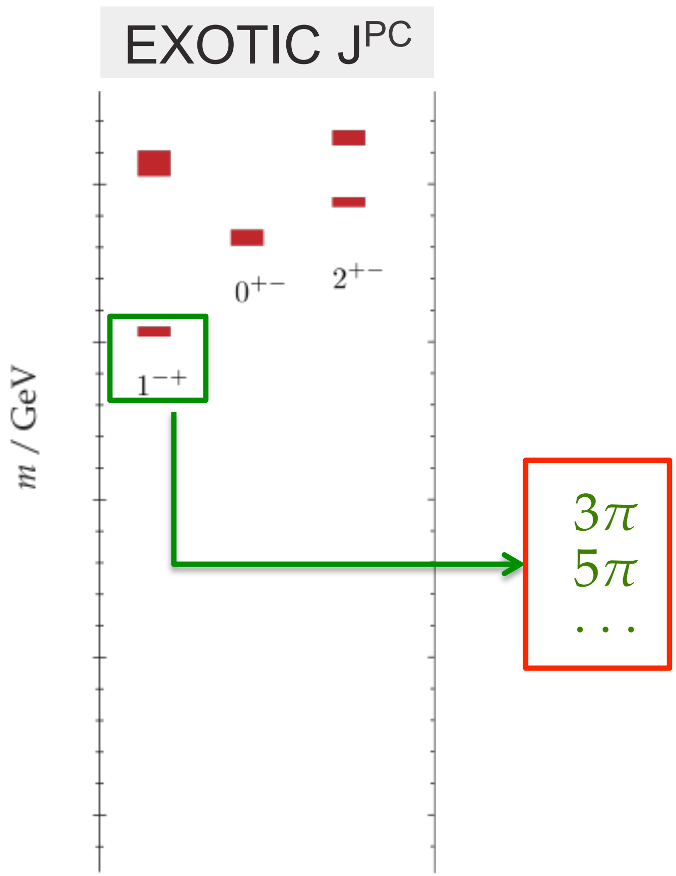
Objective by 2017

- Compute decays (branching fractions) of exotic mesons:

EXOTIC J^{PC}



Objective by 2017

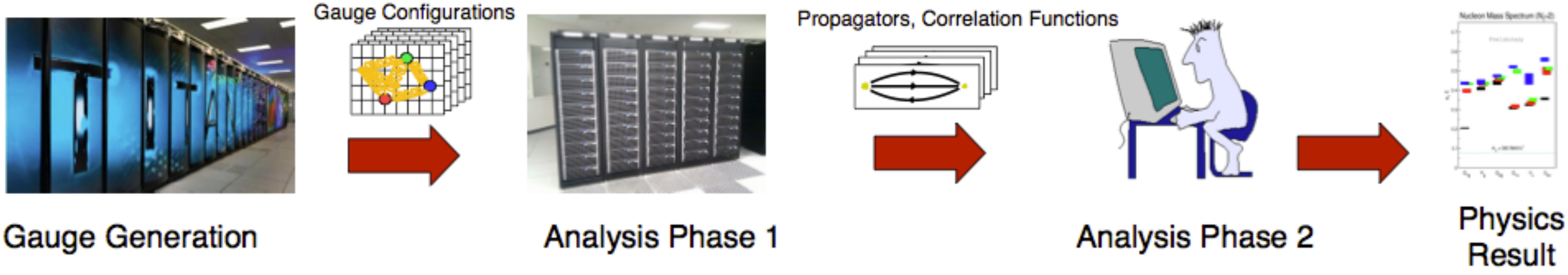


- LQCD suggests existence of exotics
- Expt. determination will require measurement in many decay channels
- Present LQCD calculations missing this info.

- Objective is to compute them ahead of expt.
- Can guide expt. analysis

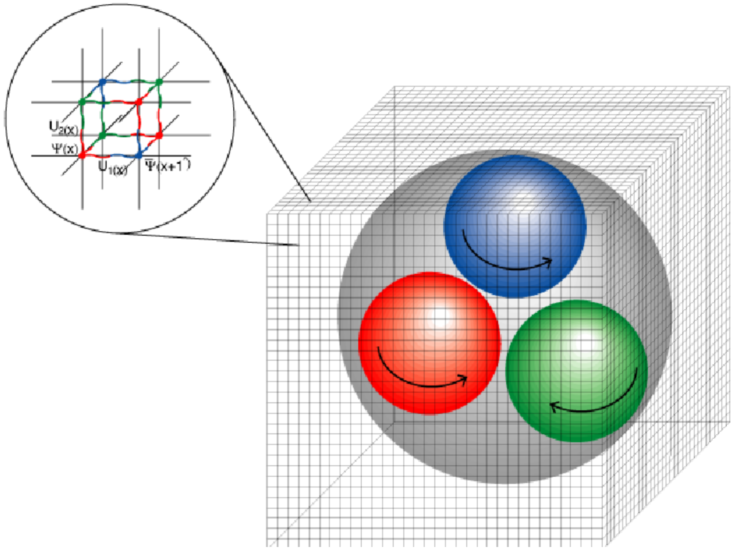
JLab Expt. beam starts in 2015 !

LQCD Calculation Workflow



- Gauge generation: capability computing on leadership facilities
  - Configurations generated in sequence using Markov chain Monte Carlo techniques
  - Focus power of leadership computing onto single task exploiting data parallelism
- Analysis: capacity computing, cost effective on clusters
  - Task parallelize over gauge configurations in addition to data parallelism
  - Can use clusters, but also LCFs in throughput (ensemble) mode

Gauge generation

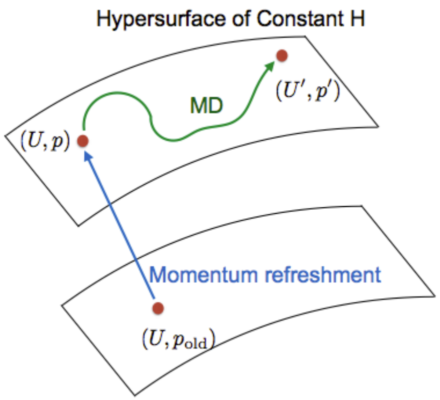


Hybrid Monte Carlo (HMC)

- Hamiltonian integrator: 1st order coupled PDE's
- Large, sparse, matrix solve per step

- "Configurations" via importance sampling
- Use Metropolis method

- Produce ~1000 useful configurations in a dataset

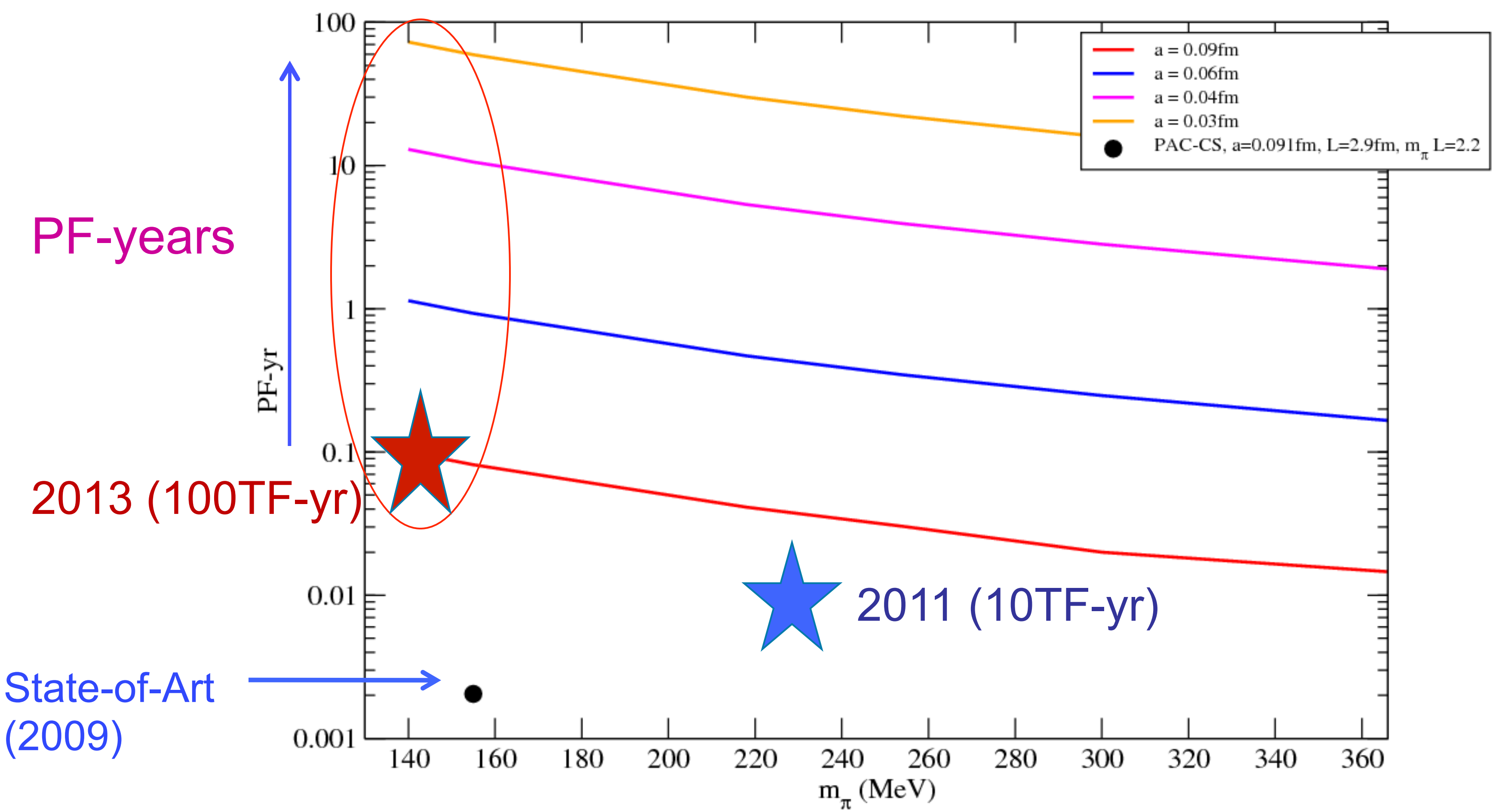


Cost:

- Controlled by lattice size & spacing, quark mass
- Requires capability resources

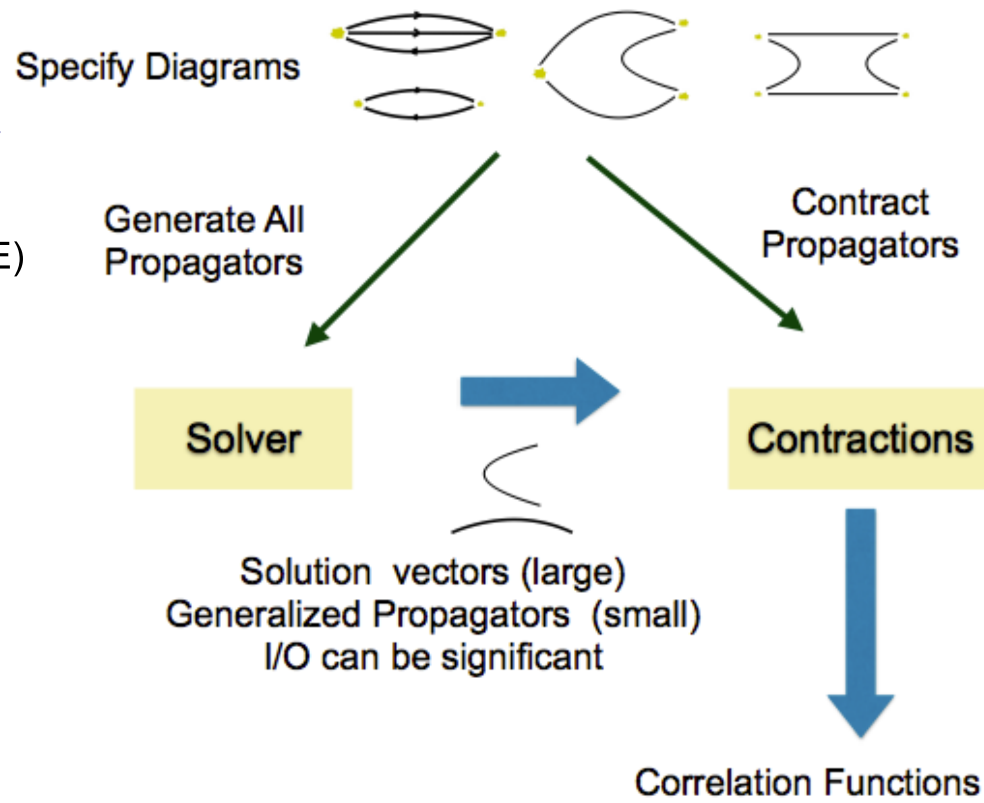
Gauge Generation: Cost Scaling

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



Analysis pipeline

- Two main components
  - Propagator calculations (solver)
  - Contraction calculations (distillation)
- Contractions use dense matrix multiply
  - Matrix dimension is O(100)
  - Considering Tensor Contraction Engine (TCE)
- Many solves needed on single config:
  - #spin x #timeslices x #sources x #quarks
- Our present largest calculation:
  - 4 spins, 256 timeslices, 384 vectors, 1 quark
  - 395,264 individual solves per configuration
  - Huge # for LQCD
  - Fast solves enable new class of algorithms
    - New ways to reduce contraction costs



NERSC + ORNL resources resources

Summary - computational strategy

Gauge generation

- Generate gauge fields using Hybrid Monte Carlo
- Solvers ~60% - 80% of run-time
  - Gauge fields (hence linear operator) changes along trajectory
- Must tune integrator parameters
- Potential research areas:
  - shadow Hamiltonians
  - Force Gradient Integrators
  - Multi-Grid in the integrator

Analysis

- Dominated by solver
  - O(10^5 – 10^6) solves per config
  - GPUs have made this possible
  - Multi-grid works well here
  - MG code on accelerators next step
- Contractions: large dense matrix multiplies
  - Scope for accelerators with BLAS libraries (CUBLAS, MKL)
- I/O bottlenecks when saving solution vectors

Summary – computational requirements

Gauge generation

- Challenges:
  - Solver cost growing (light quarks)
  - Plethora of platforms
- Scaling limitations:
  - Strong scaling solvers
    - Bottleneck is balancing memory bandwidth to comms
- Improvements (by 2017):
  - Multi-level/deflation techniques in solvers also implemented in integrator
    - More compute for each comm
  - New code generation schemes made more platform independent

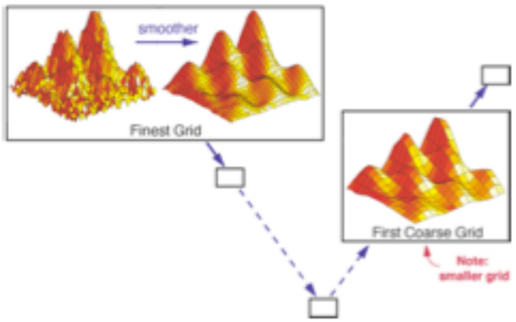
Analysis

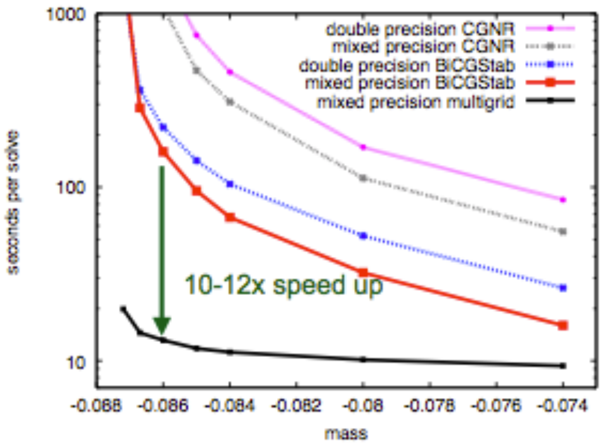
- Challenges:
  - Ever larger number of solves to achieve desired statistical precision
  - Contraction costs
- Scaling limitations:
  - Solves on small-ish number of nodes – okay
  - Limitation becoming I/O
    - Large number of concurrent solves
- Improvements (by 2017):
  - Better inverters coming on-line
  - Improved methods for contractions
  - Moving contractions to accelerators

Algebraic Multi-Grid (CPUs)

- Multi-Grid method
  - QCD: no geometric smoothness ➔ algebraic multigrid
  - Setup is costly
  - Easily amortized in Analysis with > 100 solves
- Significant impact on our program
  - See 10x improvement over our best CPU inverter
  - Room for more – multiple right-hand-sides

Image From: http://computation.llnl.gov/casc/sc2001_fliers/SLS/SLS01.html
Credit: LLNL, CASC

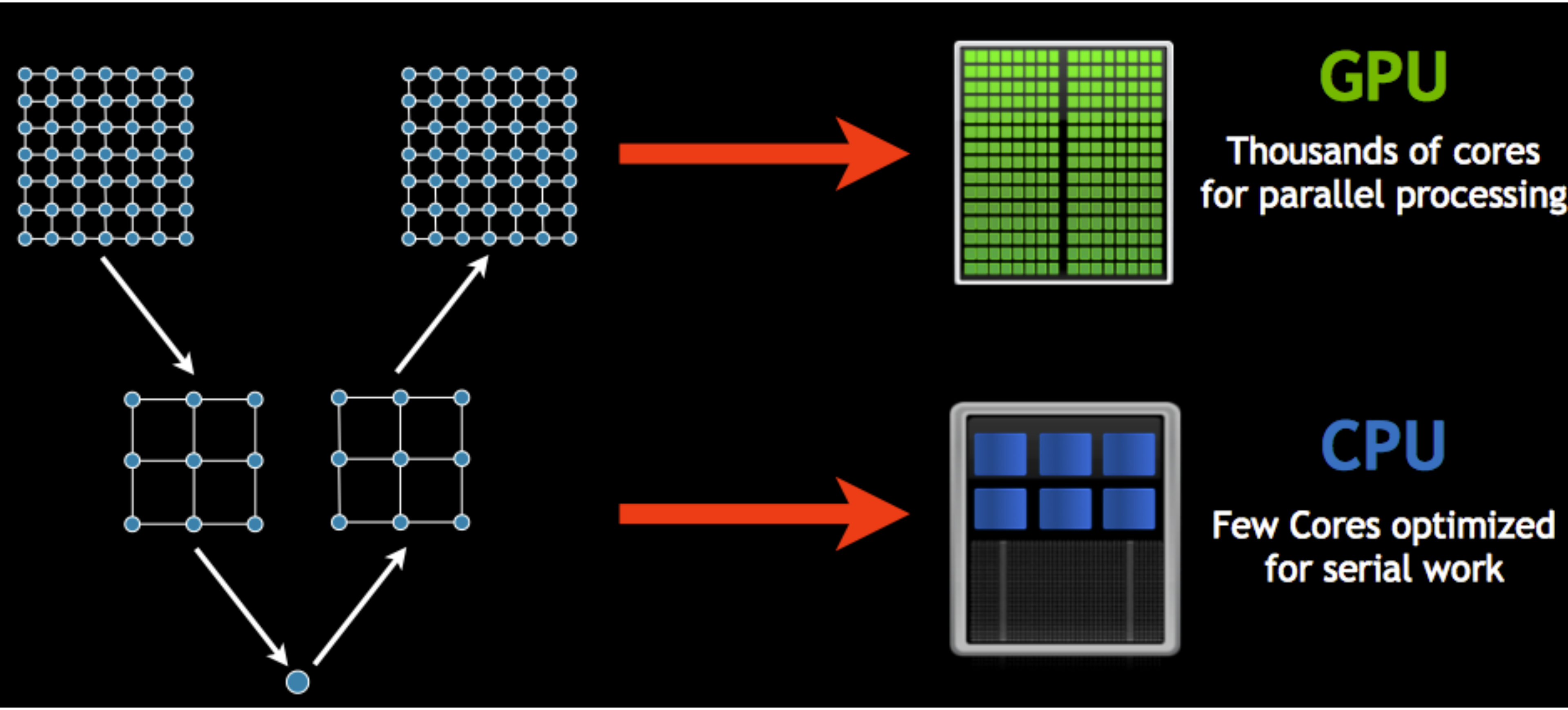




Multi-Grid. figure from J. C. Osborn et. al. PoS Lattice 2010:037,2010, R. Babich et. al. Phys. Rev. Lett, 105:201602,2010

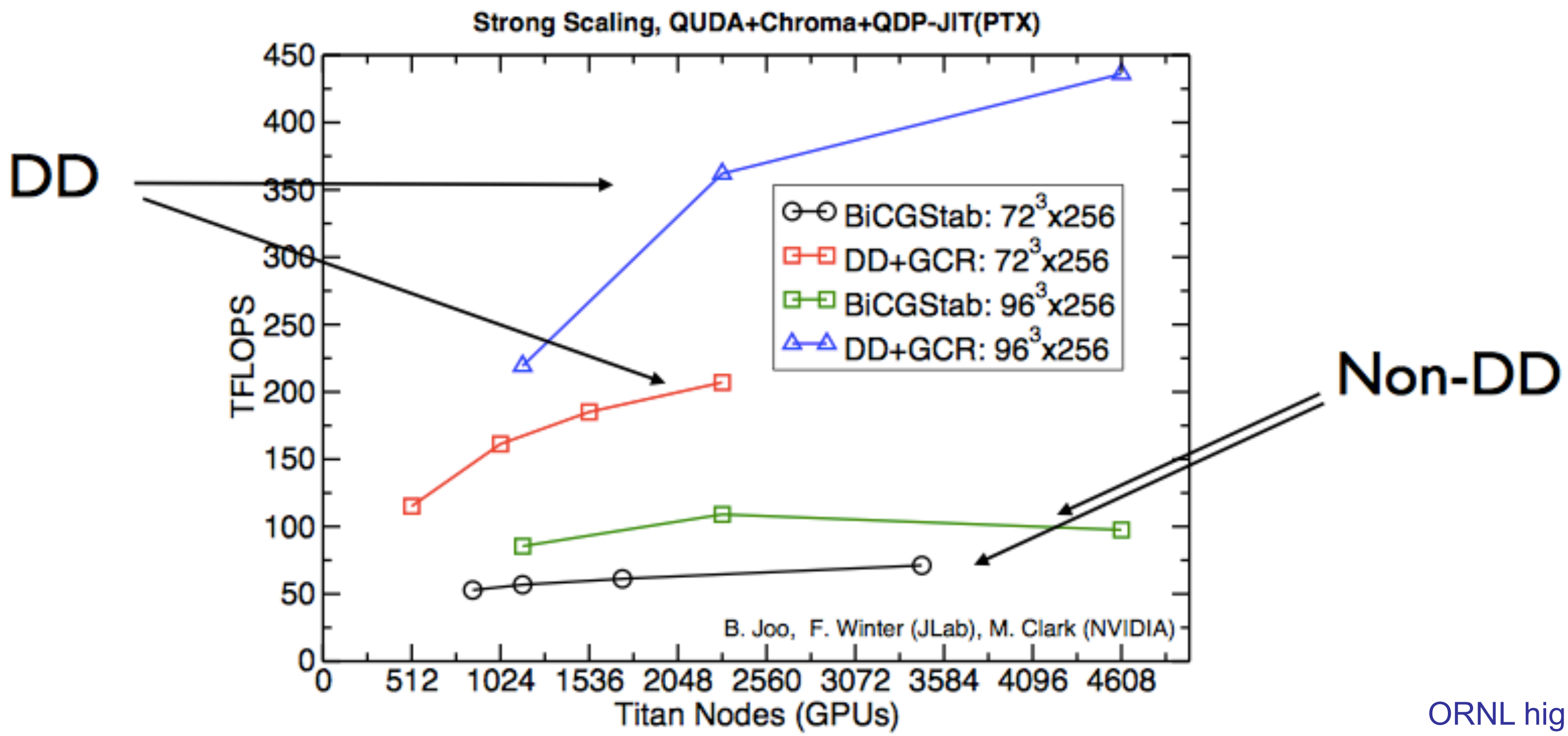
Hierarchial algorithms on heterogeneous architectures

- Extend algorithm to use different subsystems
- Lifted from M. Clark (Nvidia)



GPU solver performance

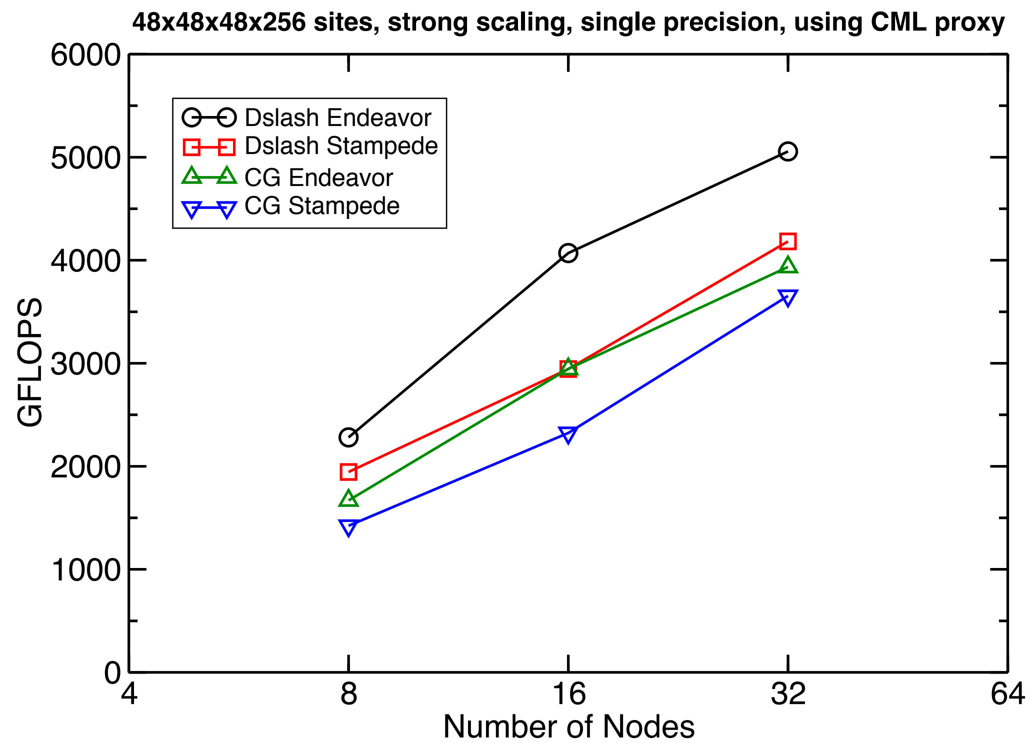
- Domain-decomposition for GPUs
  - Avoid communications
  - Significant performance increase
  - 3x or more over best GPU



ORNL highlight

Intel Xeon Phi-s

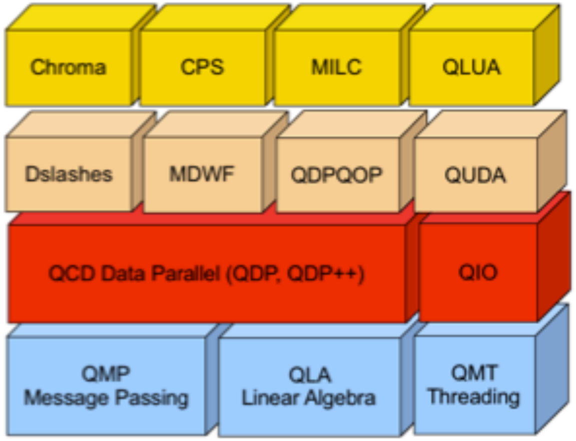
- Significant development effort
  - USQCD SciDAC, Intel Parallel Computing Labs (Santa Clara + Bangalore), Regensburg
- Stampede
  - Initial strong scaling tests
- Papers in SC’13, ICS’13, IPDPS’14



Lattice QCD on Intel Xeon Phi Processors, **B. Joo, P. Dubey, K. Vaidyanathan, M. Smelyanskiy, K. Pamnany, V. Lee, P. Dubey, W. Watson, in ICS’13**

USQCD Software Stack and Chroma

- Chroma application suite for LQCD calculations
  - Developed under US DOE SciDAC-1 and 2 initiatives
  - Used for gauge generation and analysis
  - Large worldwide user base
- General scheme
  - High level application codes (Chroma plus others)
  - Optimized libraries (e.g., for Dirac Matrix and Solvers)
  - Data parallel (productivity) level, we use QDP++
  - Portability libraries (we use primarily QMP built over MPI)



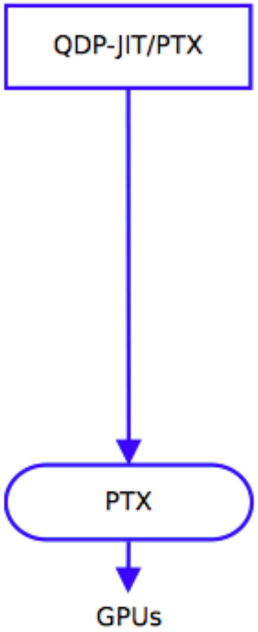
QDP++

- Data-parallel interface
  - Lattice containers, linear algebra operations, shifts and global reductions
  - Heavy use of MPI & OpenMP
  - Uses expression templates for data type composition & operations
    - Downside - evaluation can be inefficient
  - Want performance and expressibility on all platforms. How?

- Solution: back end code generator
  - Expression templates generate code generators, which then execute at run-time

QDP-JIT/PTX

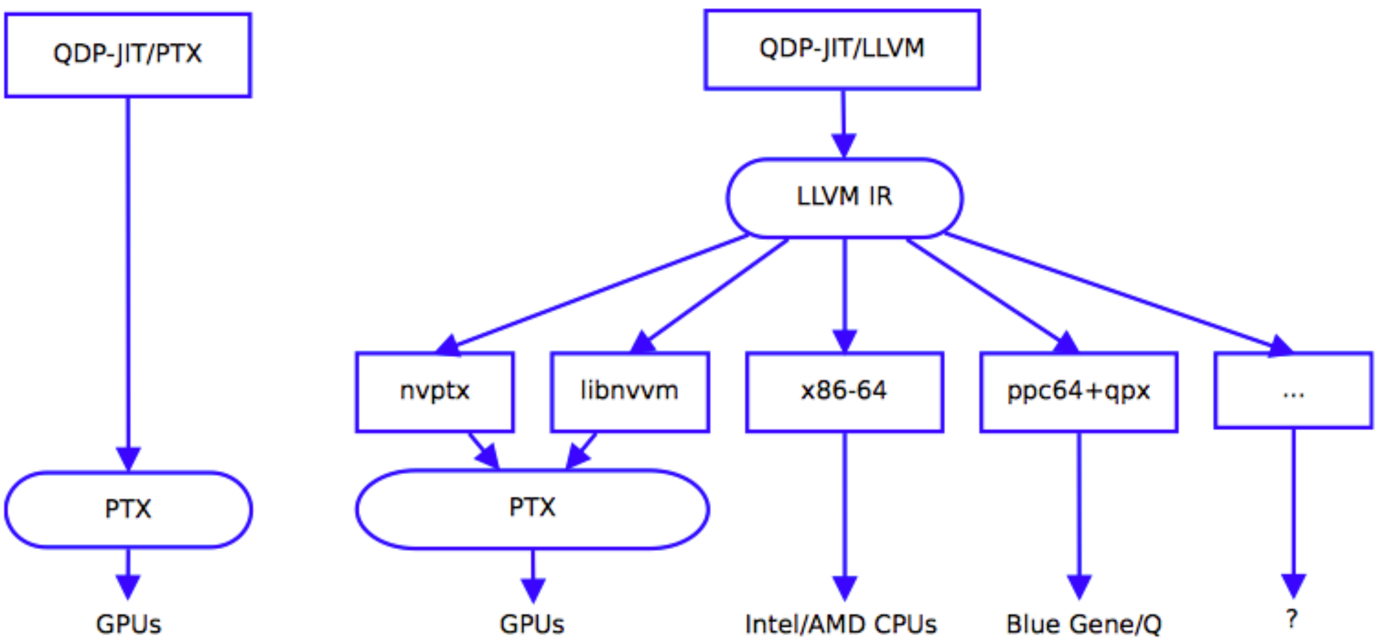
- Data-parallel interface with code generation
- GPUs
  - Expression template code runs on host
  - Generates code-generators, which generate PTX at run-time
  - Allows remapping data on the fly between host and GPU device



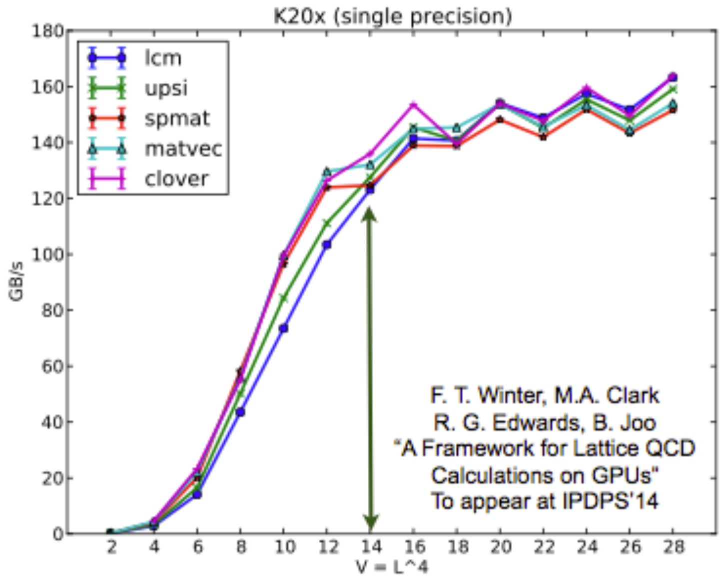
QDP-JIT/LLVM

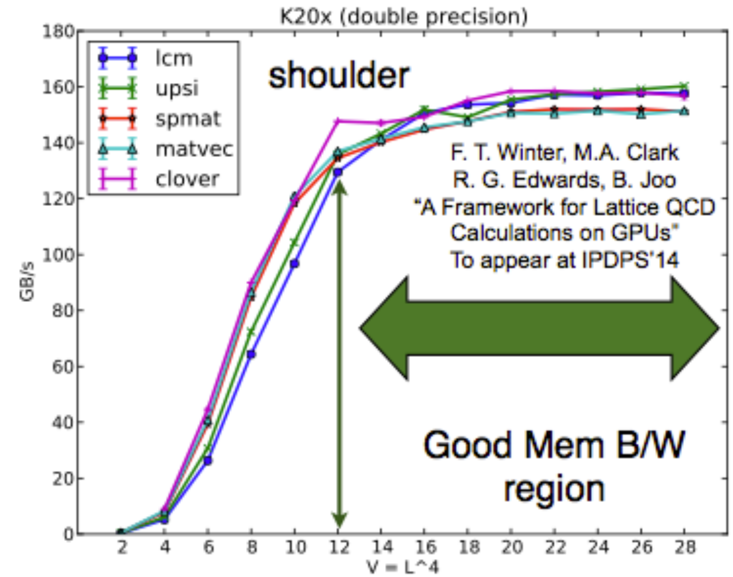
- Data-parallel interface with code generation
- CPUs, GPUs, BlueGenes, (the world…)
  - Expression template code runs on host
  - Generates LLVM Intermediate Representation (IR)
  - LLVM compiler framework has multiple back-ends, including GPUs

JLab + SciDAC Super Institute



QDP-JIT/PTX

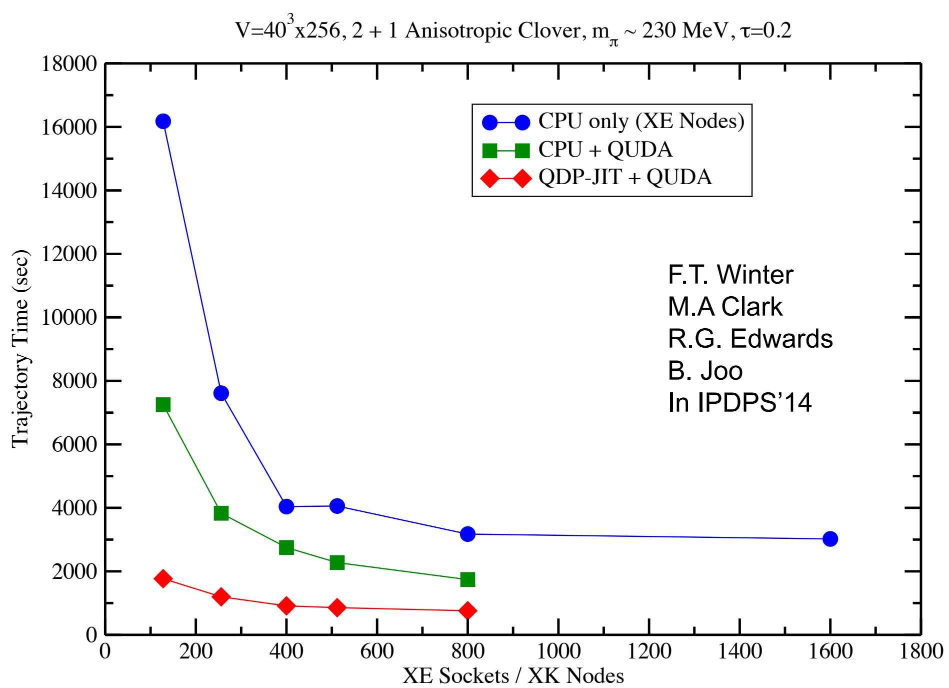




- NVIDA K20m GPUs has max Mem Bandwidth of ~180 GB/sec ECC on
- QDP-JIT/PTX achieves 150 GB/sec, ~83% of peak
- Max perf reached around 12^4 – 14^4 local lattice on single node

QDP-JIT+QUDA on Cray XK7

- Putting all the pieces together – gauge generation
  - At 128 nodes: 11x speedup
  - At 800 nodes ~3.7x speedup
  - For 40^3x256 lattice, shoulder entered around 400 GPUs
- Current production on 72^3x256 lattices – comfortably scale to 2000 GPUs



HPC usage

Gauge generation

- Machines:
  - ORNL/INCITE: 140M (2013), 58M (2014)
  - NERSC: 18M (2013)
  - NCSA/PRAC: 100M (2014)
- Parallelism:
  - 64K cores (4096 nodes)
  - # jobs ~ 1K
- Data:
  - Disk: read 50GB, write 50GB
- Software:
  - CUDA, LLVM

Analysis

- Machines:
  - USQCD: 35M (2013) (CPUs + GPUs)
  - Stampede/NSF: 18M (2013)
  - NCSA/PRAC: 50M (2014)
- Parallelism:
  - Run smaller core counts -> fill memory
  - 8 to 512 cores : capacity mode
  - 128K cores : ensemble mode
  - # jobs > 10K
- Data:
  - Disk: read up to 50GB, write up to 1 TB
  - /scratch, Global FS
- Software:
  - BLAS, CUDA

HPC requirements

Analysis 3x Gauge generation cost

Gauge generation

- By 2017:
  - 72^3x256 lattices: 200M
  - 96^3x256 lattices: 500M
- Parallelism:
  - Up to 10K GPUs or 300K cores
- Data:
  - Read/write: 150GB

Analysis

- By 2017:
  - 72^3x256 lattices: 600M
- Parallelism:
  - Contractions: < 1K cores
  - Propagators: up to 128K cores (ensemble)
- Data:
  - Write: up to 1 TB

Next generation…

- Gauge generation & analysis
  - Continue targeting Nvidia, Intel Phi, BG/Q
  - Use OpenMP, CUDA, AVX, Phi vectorization, LLVM

- A plethora of hardware & software, but not people

- Have partnerships with SciDAC SUPER & FastMath Institutes
- Have partnerships with Intel and Nvidia

- Welcome more

Hadron spectrum collaboration

JEFFERSON LAB

Jozef Dudek
Robert Edwards
Balint Joo
David Richards
Frank Winter

TRINITY COLLEGE, DUBLIN

Mike Peardon
Sinead Ryan

TATA, MUMBAI

Nilmani Mathur

CAMBRIDGE UNIVERSITY

Christopher Thomas

U. OF MARYLAND

Steve Wallace

MESON SPECTRUM

PRL103 262001 (2009) $I=1$
PRD82 034508 (2010) $I=1,\ K^\star$
PRD83 111502 (2011) $I=0$
JHEP07 126 (2011) $c\bar{c}$
PRD88 094505 (2013) $I=0$
JHEP05 044 (2013) $D,\ D_s$

BARYON SPECTRUM

PRD84 074508 (2011) $(N,\Delta)^\star$
PRD85 054016 (2012) $(N,\Delta)_{\mathrm{hyb}}$
PRD87 054506 (2013) $(N\ldots\Xi)^\star$
arXiv:1307.7022 (2013) $\Omega^\star_{ccc}$

HADRON SCATTERING

PRD83 071504 (2011) $\pi\pi\ I=2$
PRD86 034031 (2012) $\pi\pi\ I=2$
PRD87 034505 (2013) $\pi\pi\ I=1,\ \rho$

"TECHNOLOGY"

PRD79 034502 (2009) lattices
PRD80 054506 (2009) distillation
PRD85 014507 (2012) $\vec{p}>0$