WILL DETMOLD

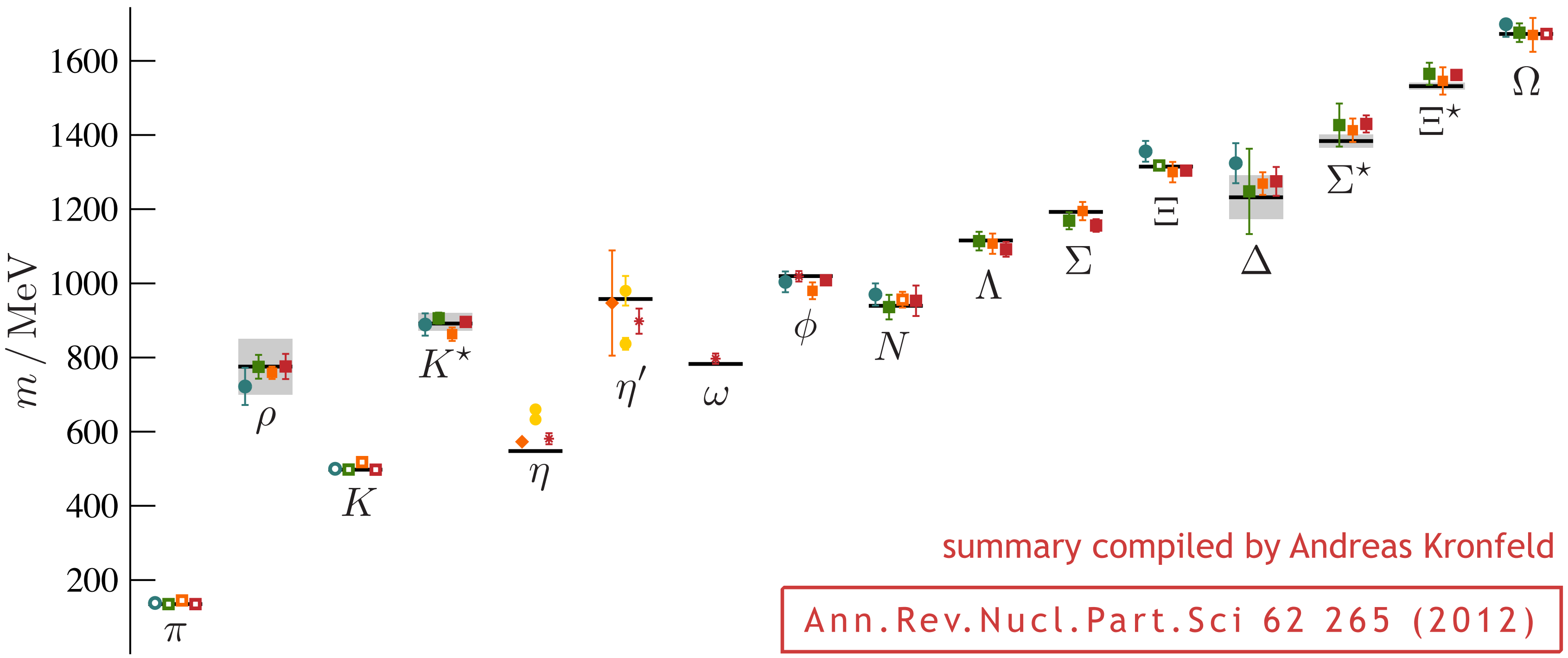
Massachusetts Institute of Technology

COMPUTATIONAL QCD: PART 2

Computational NP Town Hall 2022, Washington DC, Sep 6th, 2022

Hadron spectroscopy

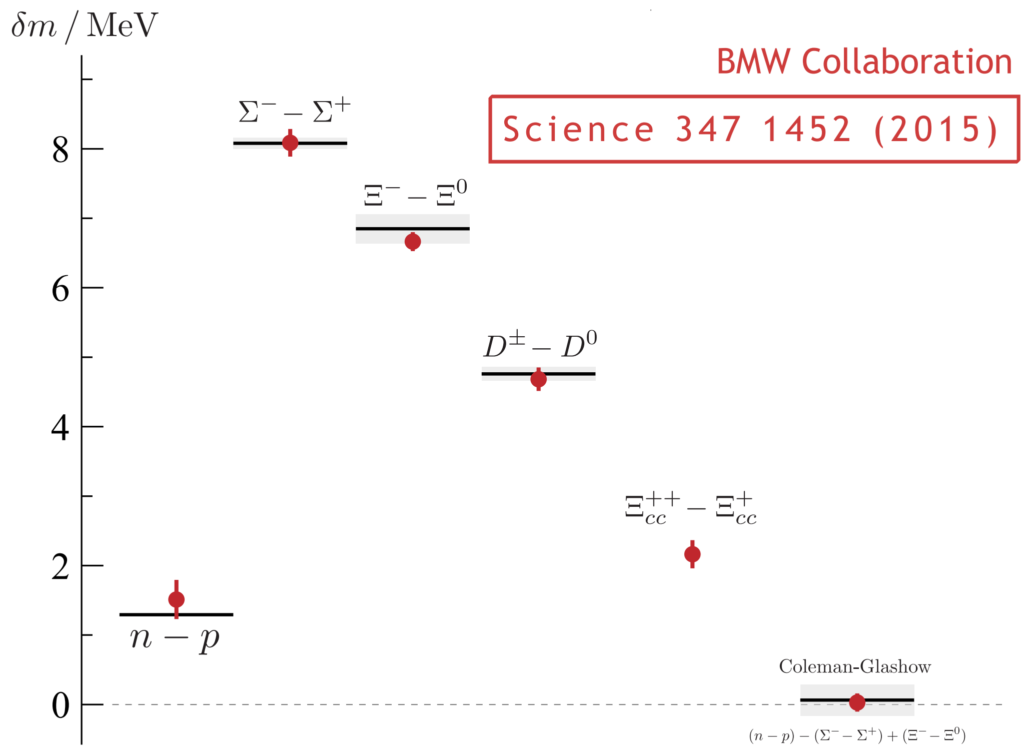
Lattice QCD stable hadron spectrum



- State-of-the-art LQCD reproduces the light stable hadron spectrum

Hadron spectroscopy

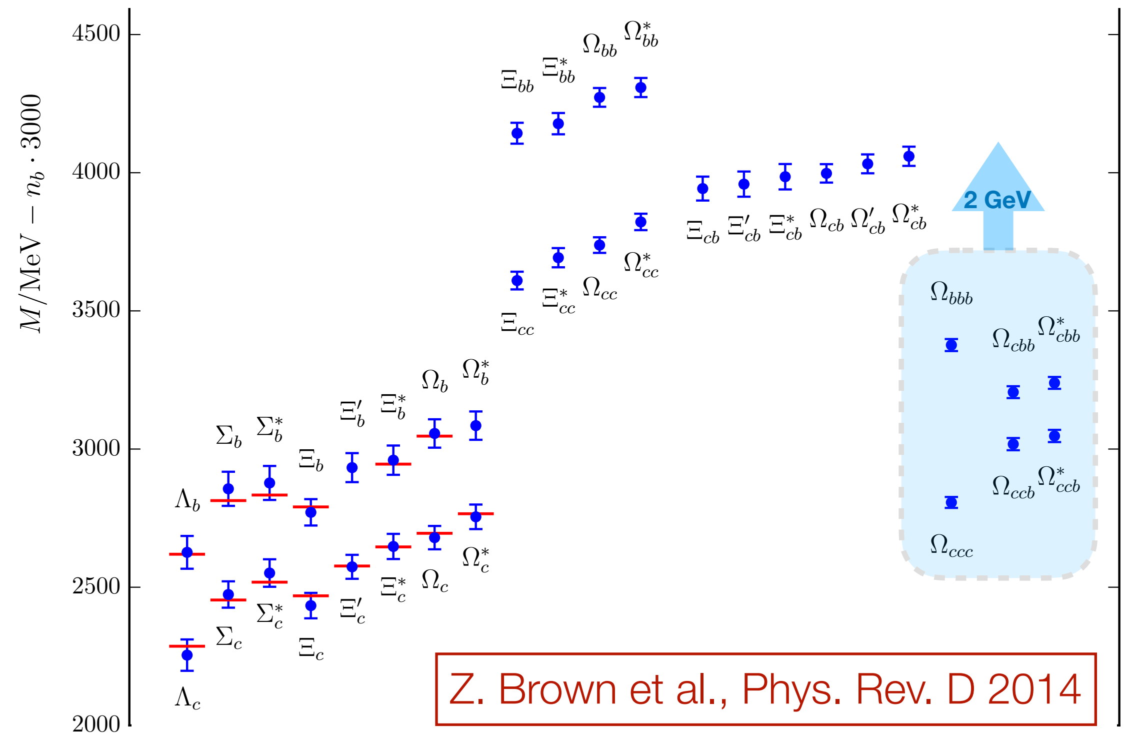
Lattice QCD stable hadron spectrum



- State-of-the-art LQCD reproduces the light stable hadron spectrum
- Separates EM and strong mass splittings

Hadron spectroscopy

Lattice QCD stable hadron spectrum



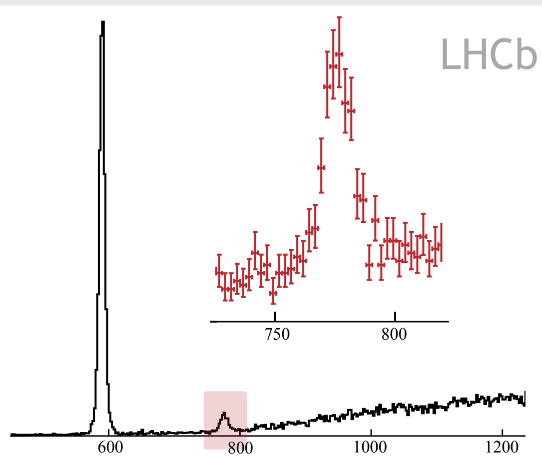
- State-of-the-art LQCD reproduces the light stable hadron spectrum
- Separates EM and strong mass splittings
- Predicted new heavy-flavoured states before experiment

SUCCESS?

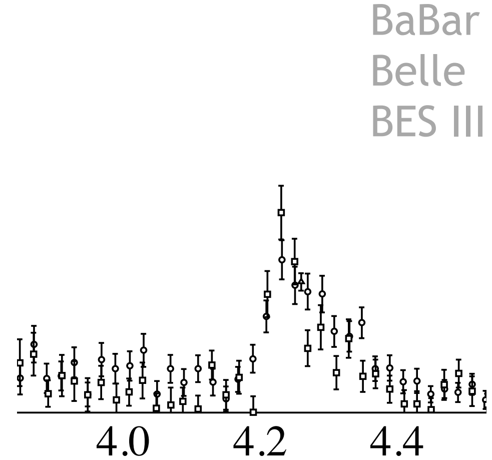
Hadron spectroscopy

Unexpected, unexplained and missing states

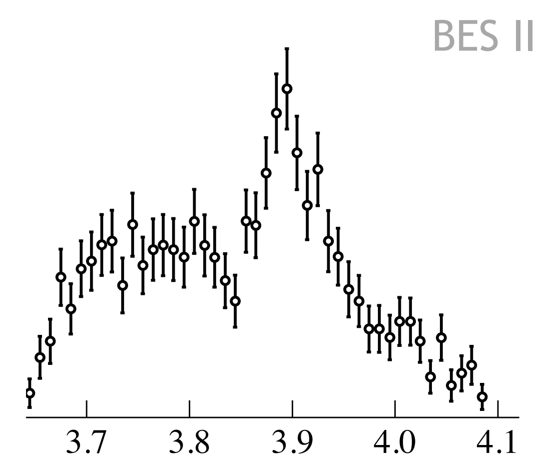
$X(3872) \to \pi\pi J/\psi$

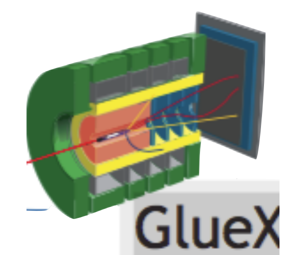


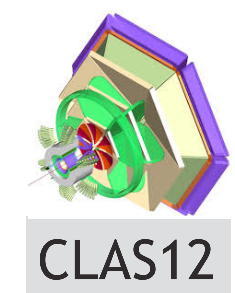
$Y(4260) \to \pi\pi J/\psi$



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





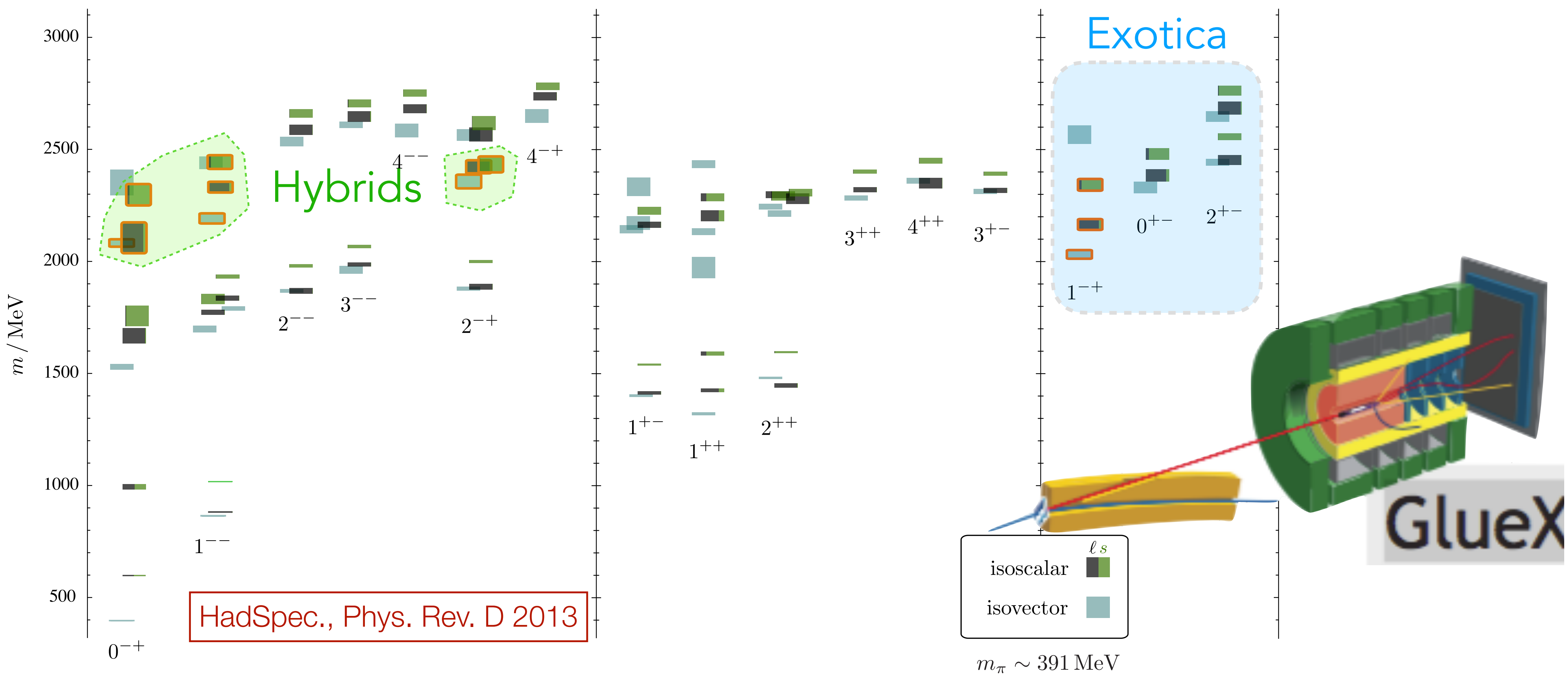


- Many new unexpected states states seen in the last two decades
- The nature of even well-known states is not well understood
- Predicted states not seen in experiment

Worldwide experimental program on spectroscopy

Hadron spectroscopy

Hybrid mesons and baryons

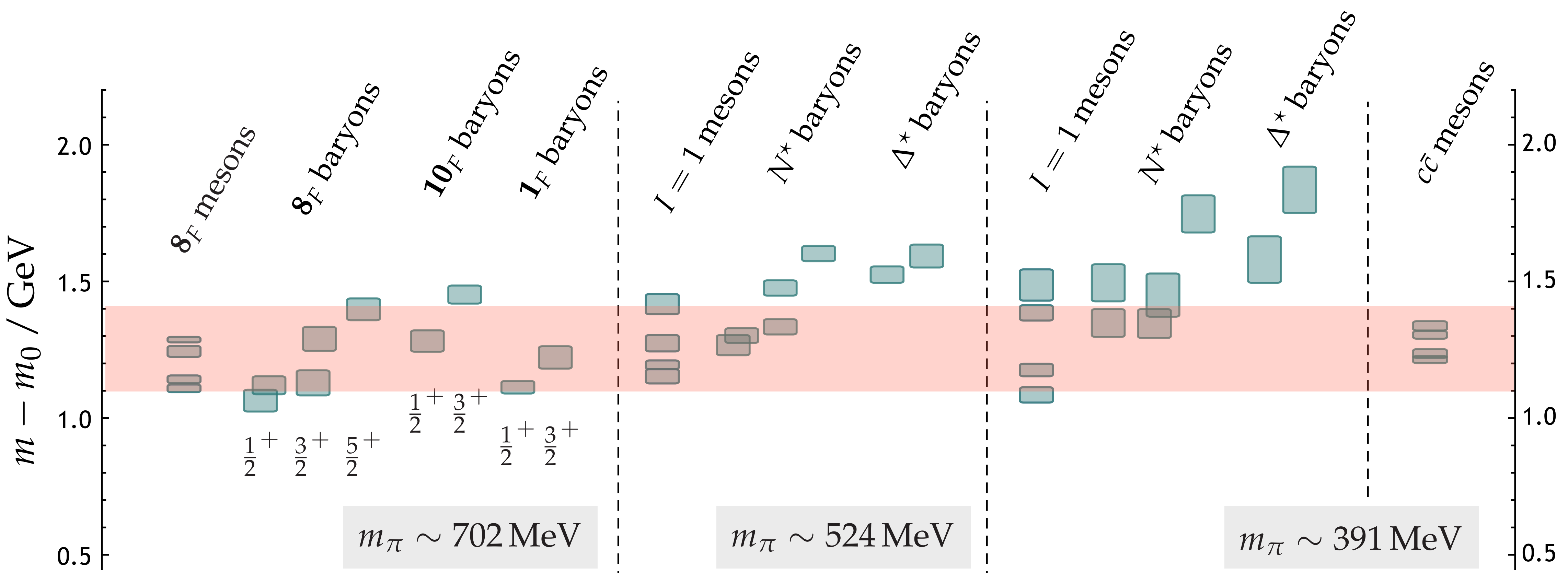


- Clear evidence for meson states that are quark-gluon hybrids or have exotic quantum numbers

Enabled by early adoption of GPUs in LQCD

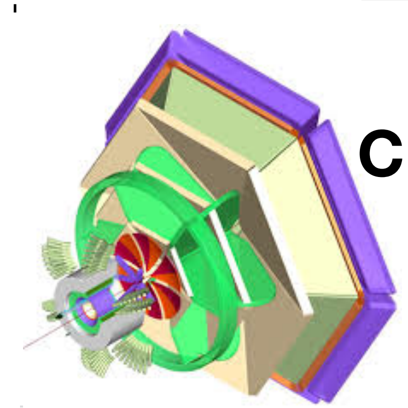
Hadron spectroscopy

Hybrid mesons and baryons



HadSpec., Phys. Rev. D 2014

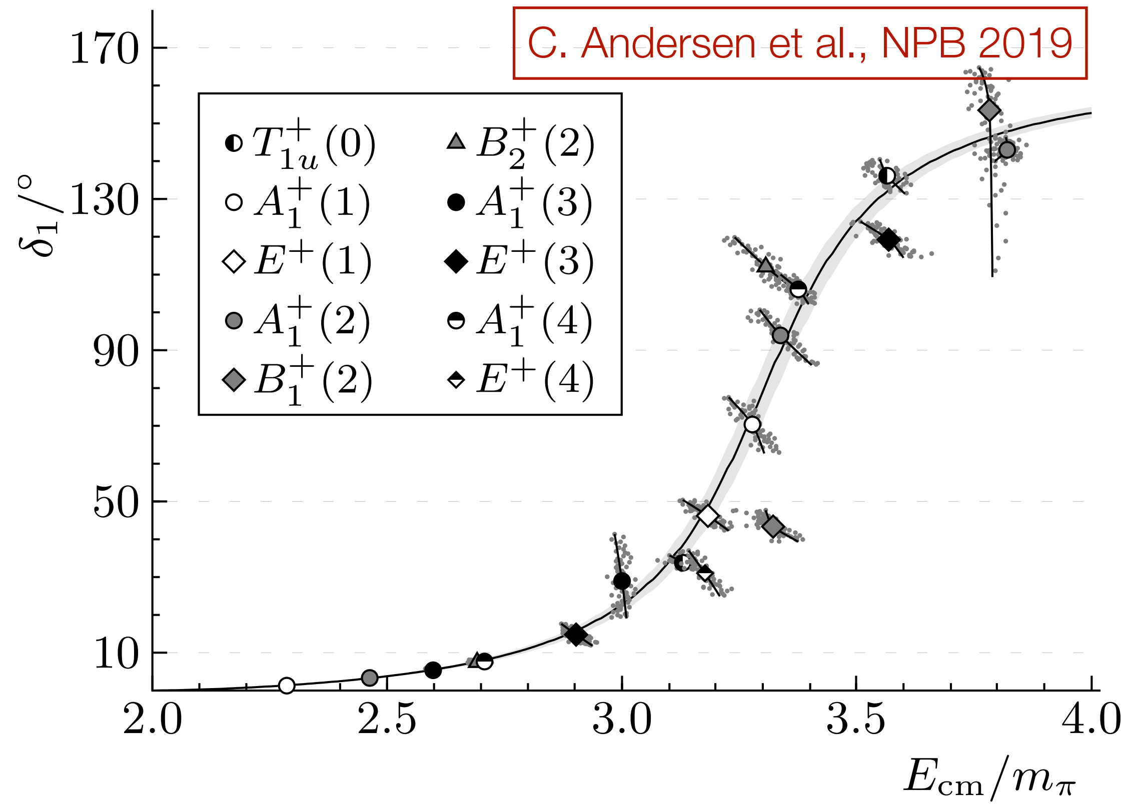
- Identified common scale for gluon excitation amongst mesons and baryons



Hybrid baryons spurred new experimental effort

Hadron spectroscopy

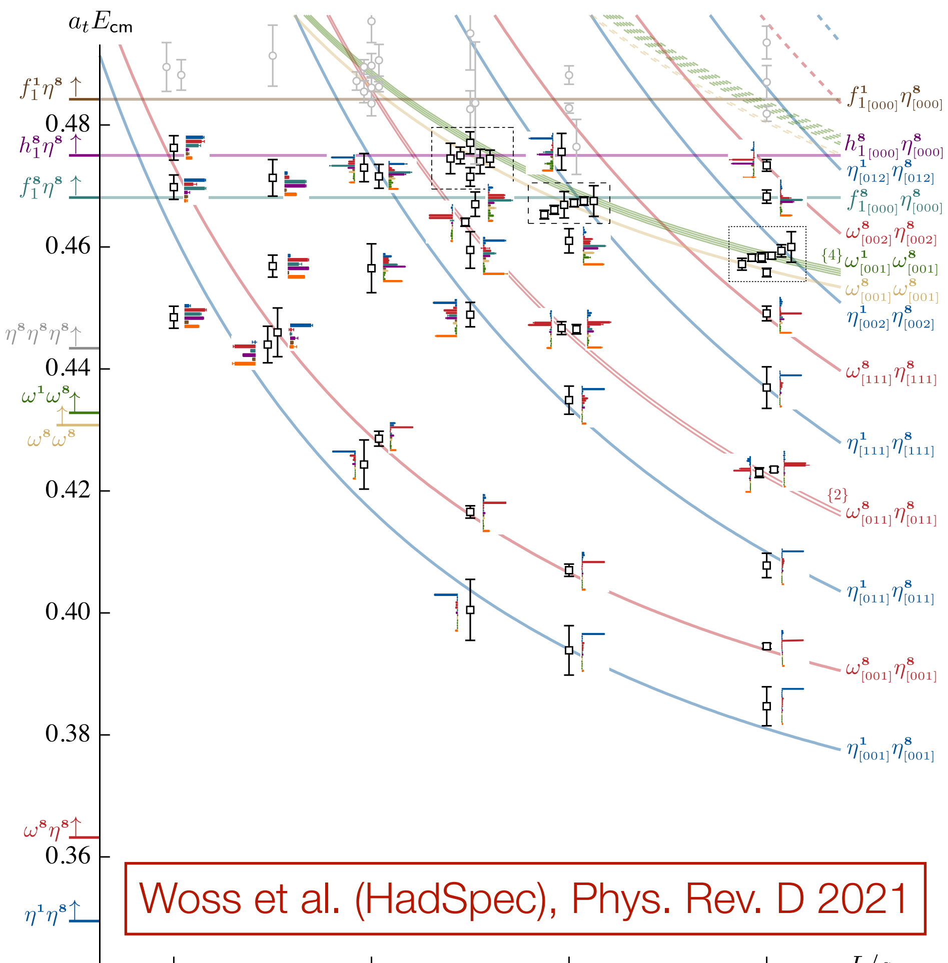
Resonant structures accessible: ρ



- Lüscher formalism maps energies from FV LQCD to scattering amplitudes
- Sophisticated implementations allow access to phase shifts and resonances
- Formalism extended to 3-body systems over the last few years

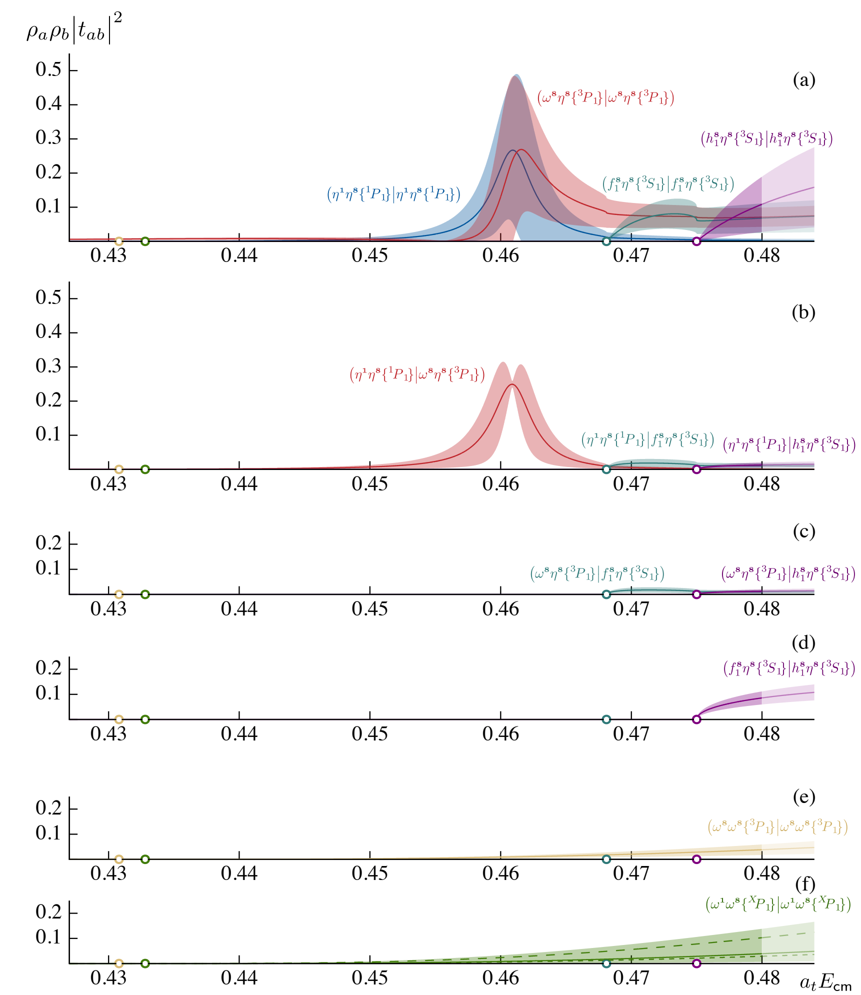
Hadron spectroscopy

State-of-the-art: exotic π_1 decays



Woss et al. (HadSpec), Phys. Rev. D 2021

63 energy levels in 4 volumes to extract scattering amplitude and decays between 8 channels!

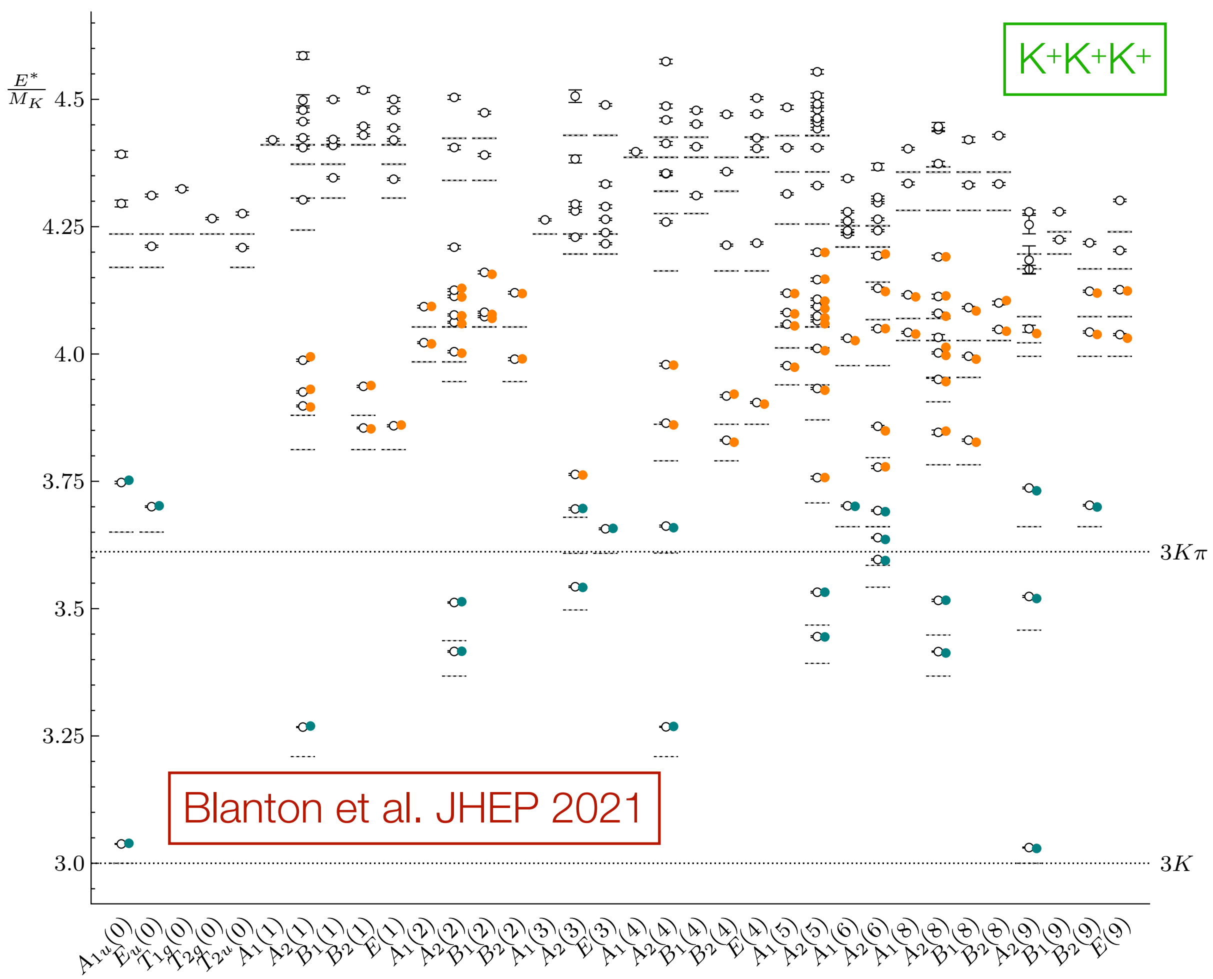


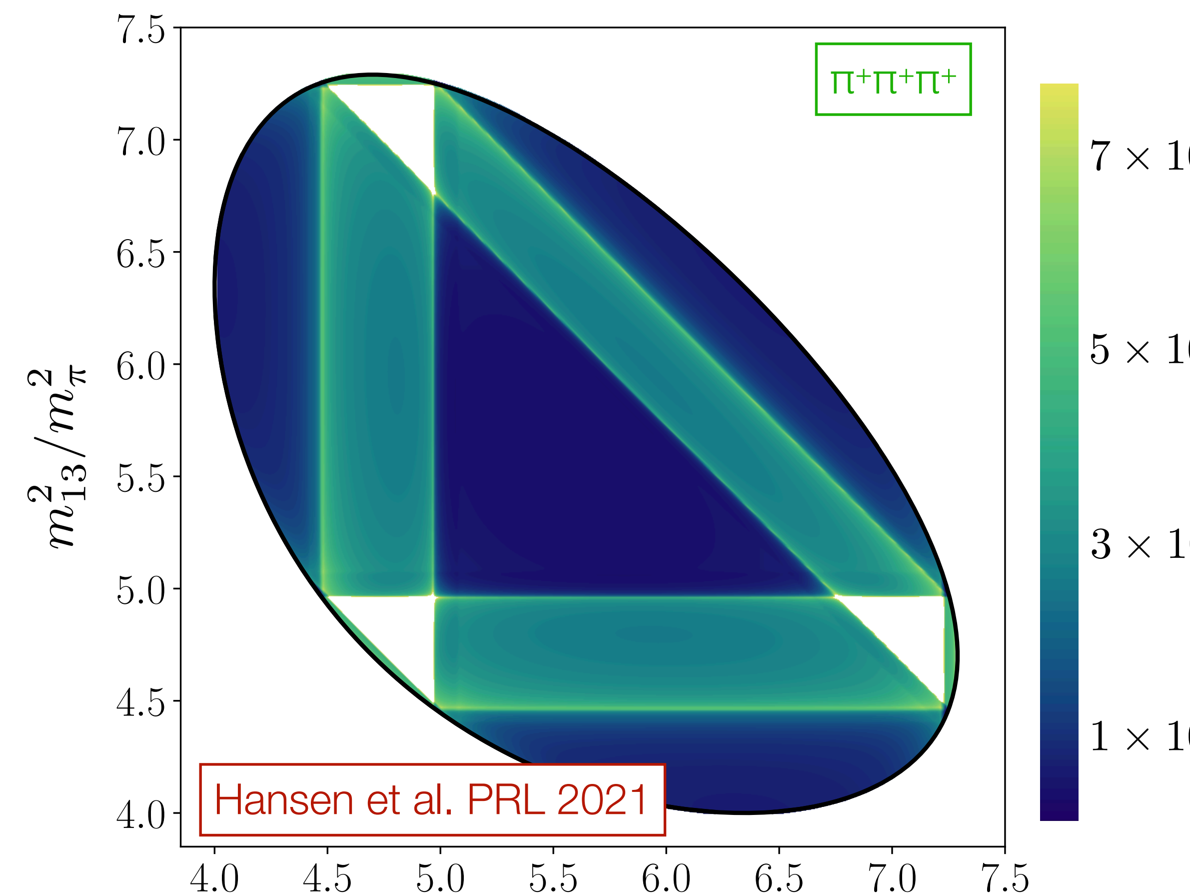
- First ever study of full decay of exotic: π_1 is a broad resonance
- Surprising decay patterns: suggests new GlueX search strategy

Required significant computation for amplitude extraction

Hadron spectroscopy

Pushing the frontier: three-body decays





- Develop technology for more complex systems such as a_1, Roper
- Determination of 3-particle amplitude (and future 3 particle decays)

Contraction costs increase rapidly - needs CS input

Hadron spectroscopy

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Computing also critical in amplitude analysis
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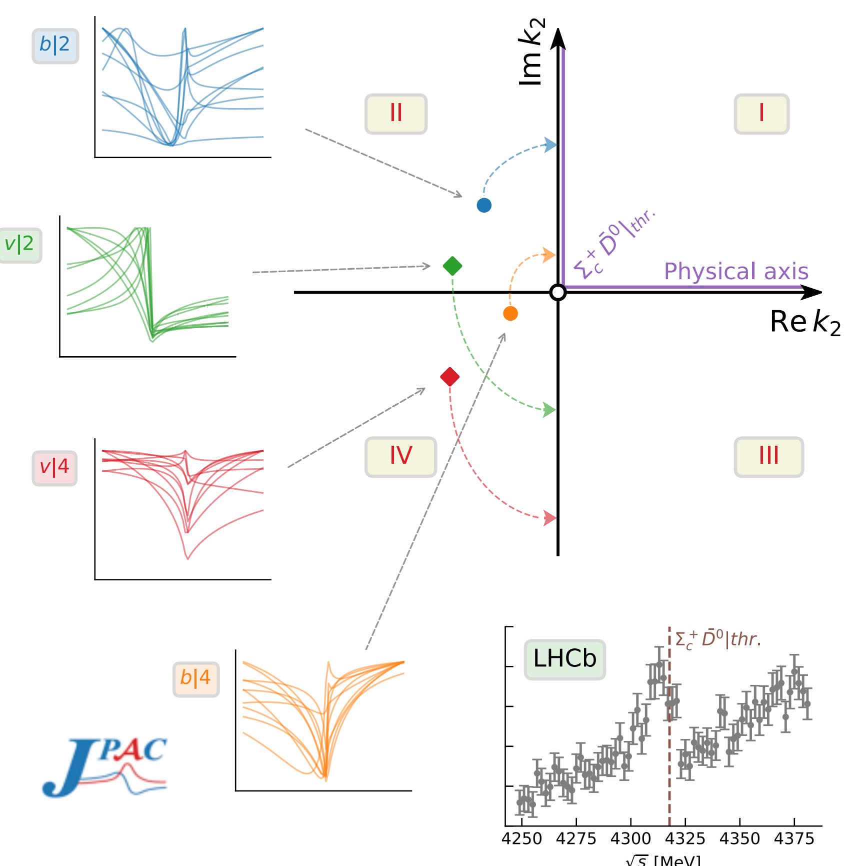
- Amplitude analysis is large scale optimisation problem
  - 100s of parameters, millions of data in multidimensional kinematic space
  - Near future: combining different datasets
- Event level analysis suitable for GPUs
- Costs ~10M CPU core hours/year + GPU
- AI/ML increasingly useful in workflows
- Workforce is key and is a limiting factor

Potential Riemann sheet structure near $\Sigma_c D$ threshold



Ng et al. (JPAC), Phys. Rev. D 2022

Computational-skilled researchers needed throughout NP

Physics of nuclei

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Baryon-baryon scattering
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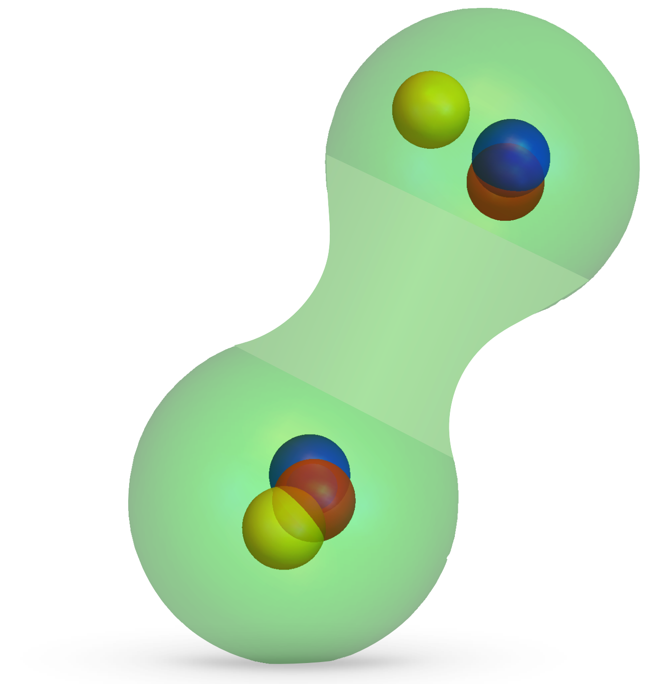
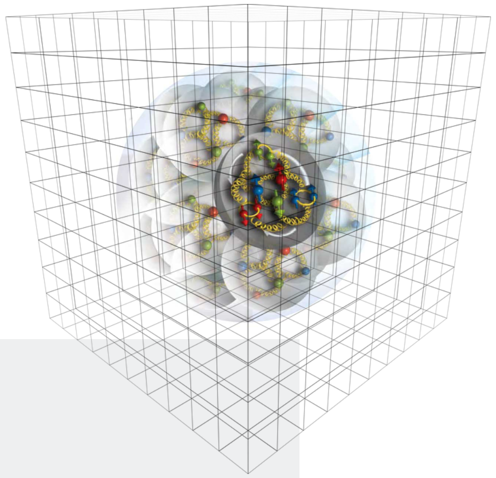
- Fully controlled connection between QCD and nuclear physics will be realised in the coming decade of exascale computing
- First calculations of BB (and A<5) systems
    - Interesting qualitative results (eg. large Nc)
    - Discrepancies in interpretation (not data) by different groups in unphysical systems *must* be addressed
    - Independent studies crucial even at unphysical point
- Exciting opportunity to address physics of hyperons in dense matter

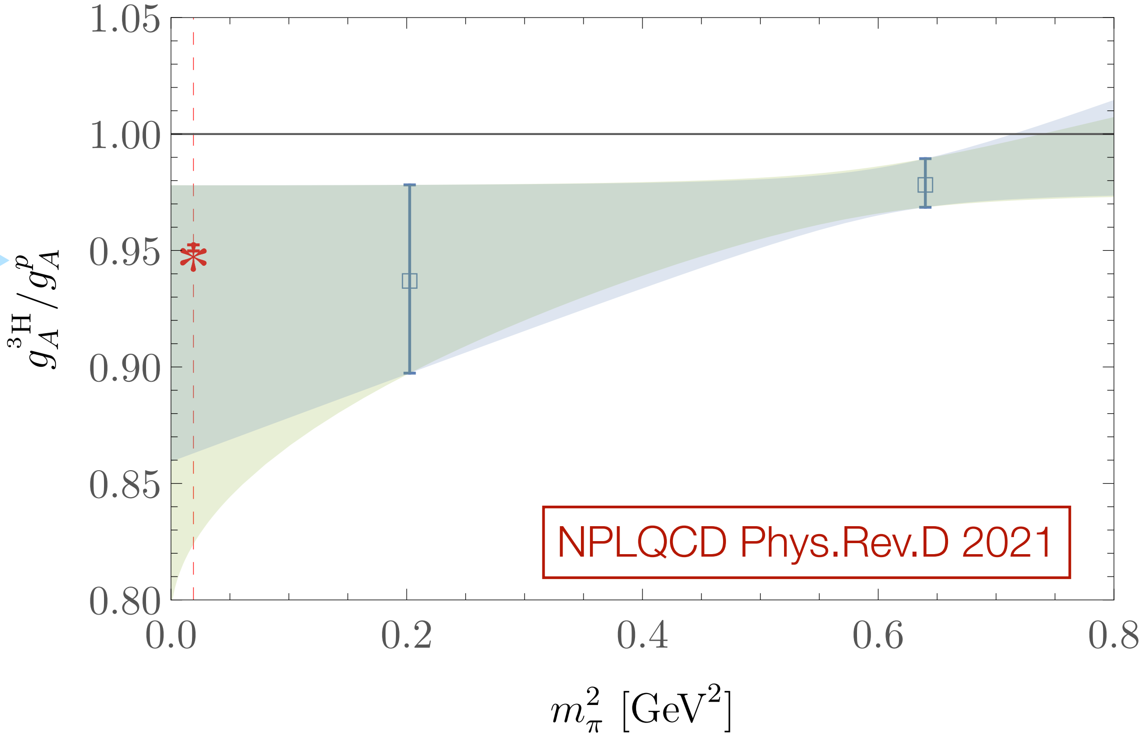


Physics of nuclei



Proof-of-principle nuclear structure

- First unphysical calculations of many aspects of nuclear structure
  - Magnetic moments & polarisabilities
  - Quenching of axial charge
  - Scalar and tensor currents
  - EMC effects: nuclear PDFs
- Nuclear processes: pp fusion and slow neutron capture
- Next decade will capitalise on these developments



Connection to larger nuclei through EFT

Fundamental symmetries

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QCD input for symmetry tests and BSM searches
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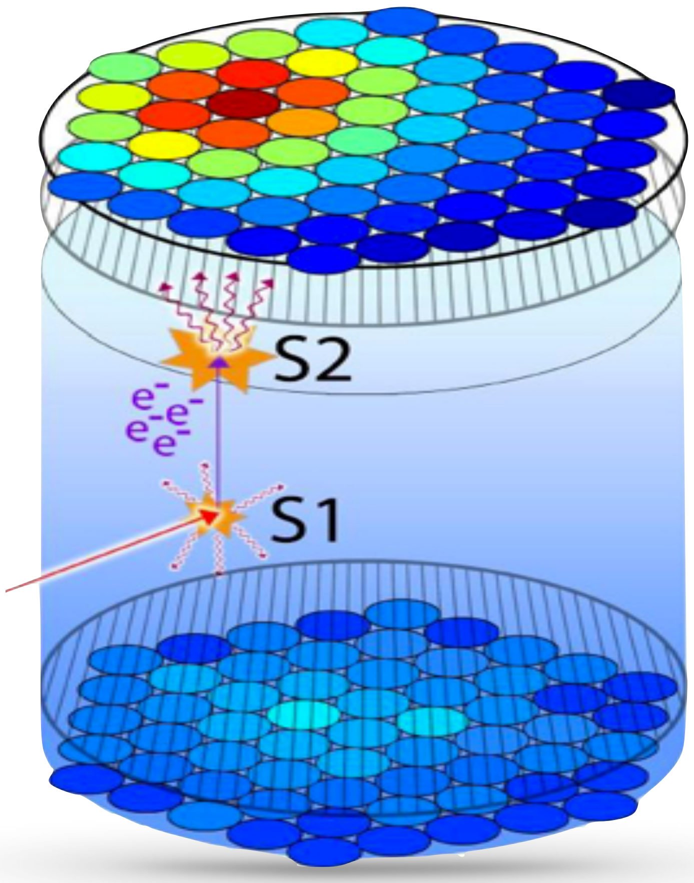
- Nuclear matrix elements needed to interpret experiments
  - Dark matter direct detection
  - Charged lepton flavour violation
  - Double beta decay
  - Proton decay, n-nbar oscillations
  - Long baseline neutrino experiments
  - EDM searches
  - and more …

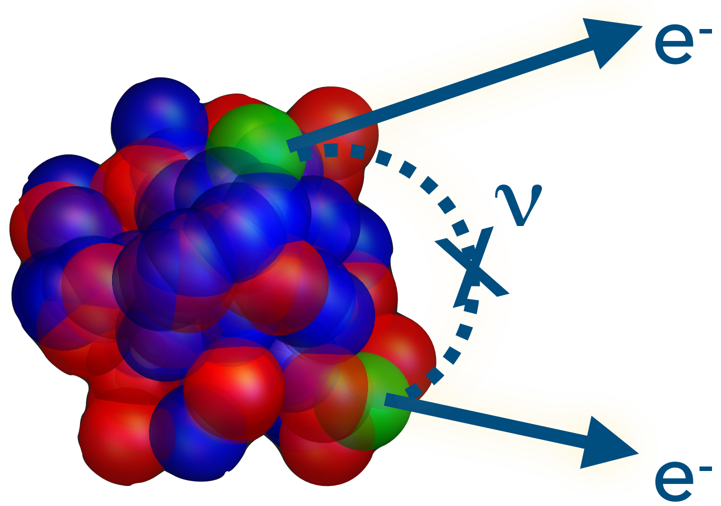


http://www.hep.ucl.ac.uk/darkMatter/

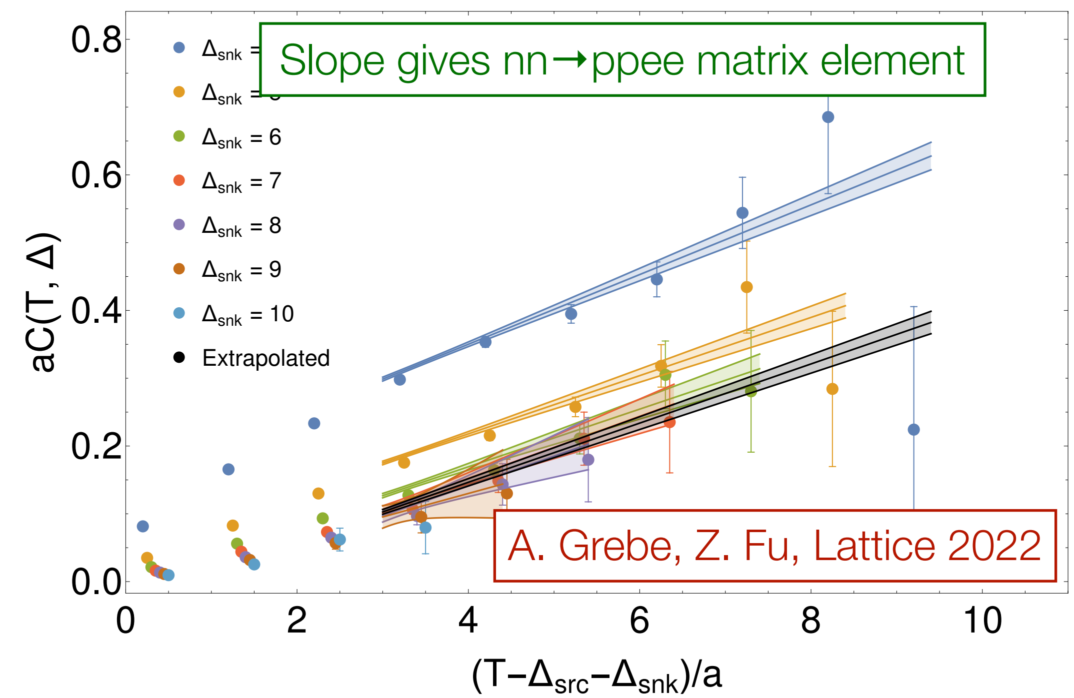
Emanuele Mereghetti will cover in his talk

Double beta decay

Expanding the horizons: second order processes



Neutrinoless double β-decay



- Matrix elements critical for DBD rates but currently model dependent
- Simplest nuclear process: nn→ppee provides QCD input for EFT
- Recent work tackles the complicated set of contractions with two electroweak current insertions

Code optimisations: previously impractical calculation now possible

Computational advances

Supported by SciDAC and ECP

SciDAC
Scientific Discovery through Advanced Computing

EXASCALE COMPUTING PROJECT

20 years of software advances

SciDAC 1&2: NP+HEP+ASCR

SciDAC 3: NP+ASCR, HEP+ASCR

SciDAC 4: NP+ASCR

SciDAC 5: NP+ASCR, HEP+ASCR ?

Readiness for exascale

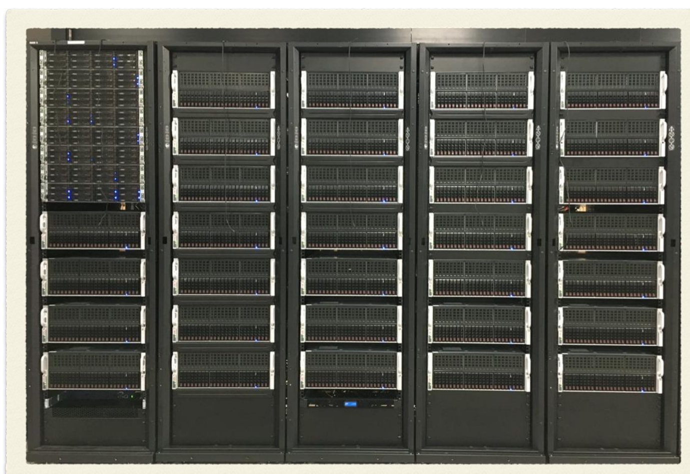
2017-now: ASCR

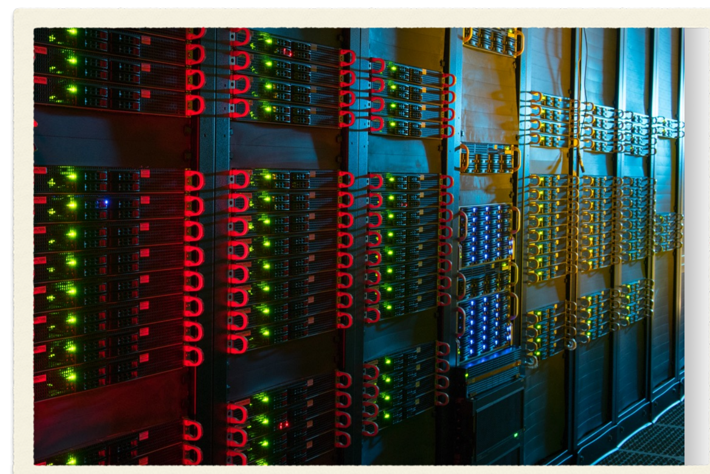
Also facility programs such as Aurora21ESP, NESAP,…

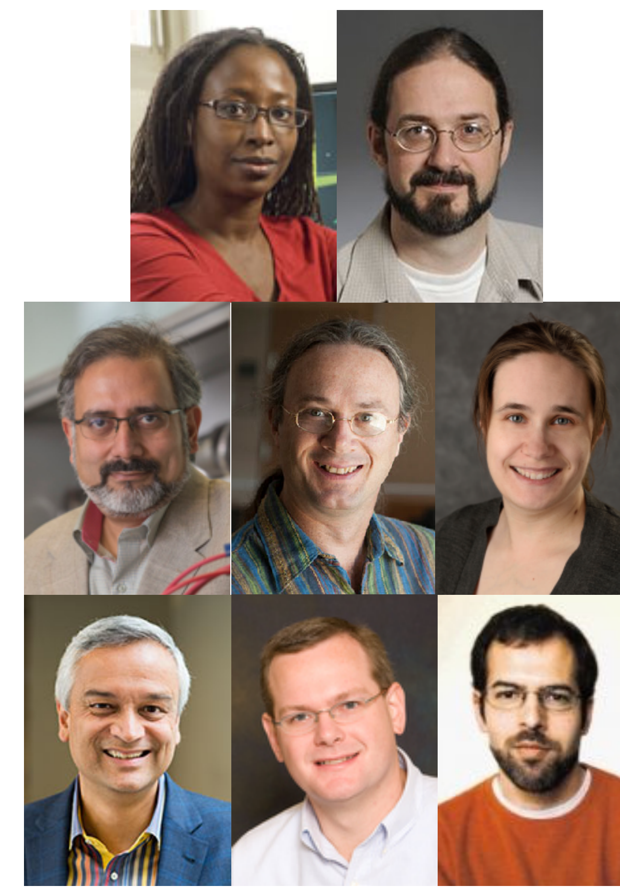
Programs vital for maintenance and extension of software stacks and hardware

Computational advances

and by LQCD project (NP + HEP)







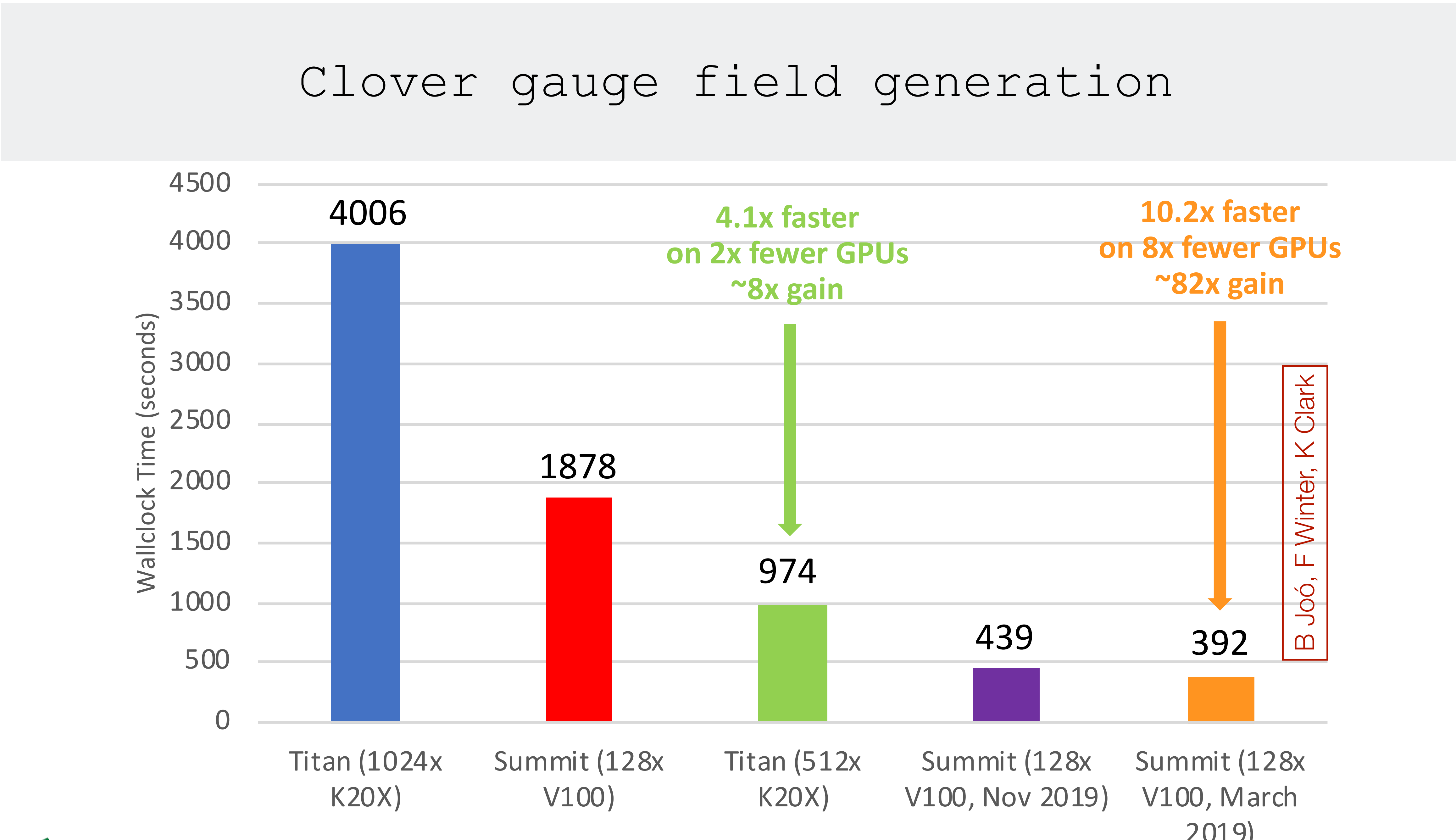
- LQCD/NPPLC projects (2001-present) have provided dedicated capacity computing for LQCD
- Managed through annual+ USQCD call for proposals
- Enables rapid exploration and development of new science goals and empowers junior investigators
- Provides ~20% of US LQCD computing

Science Advisory Board: external experts from theory and experiment

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

ASCR Leadership Computing Challenge ALCC

Computational advances

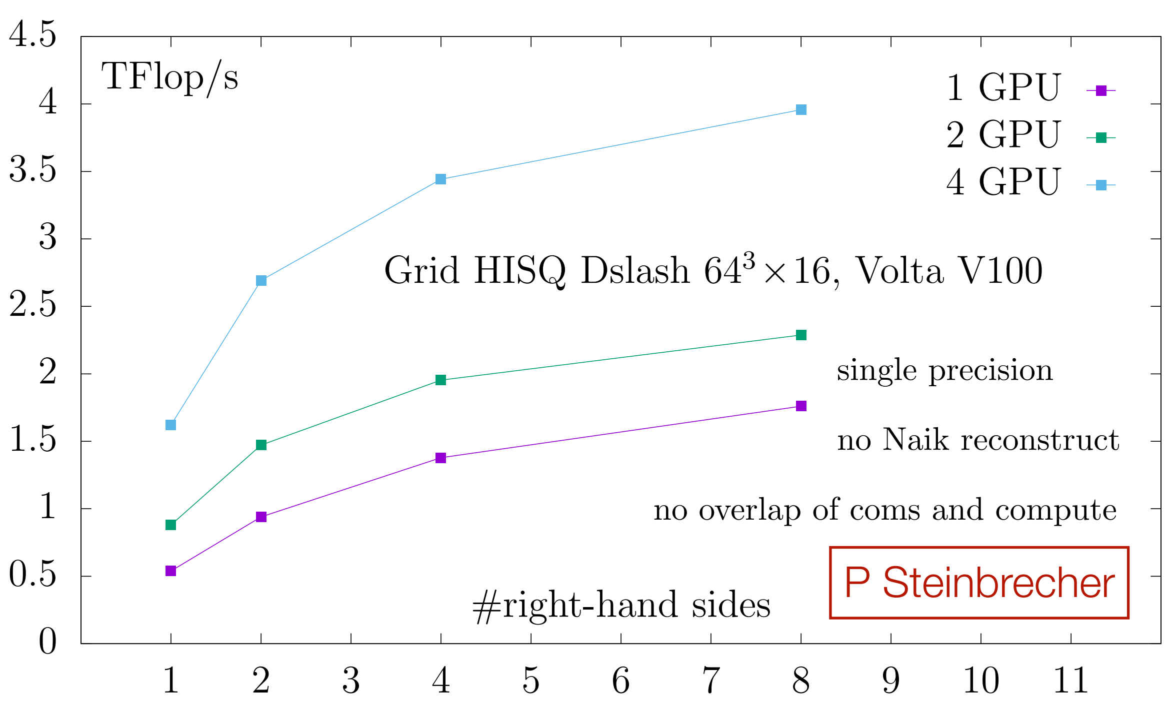


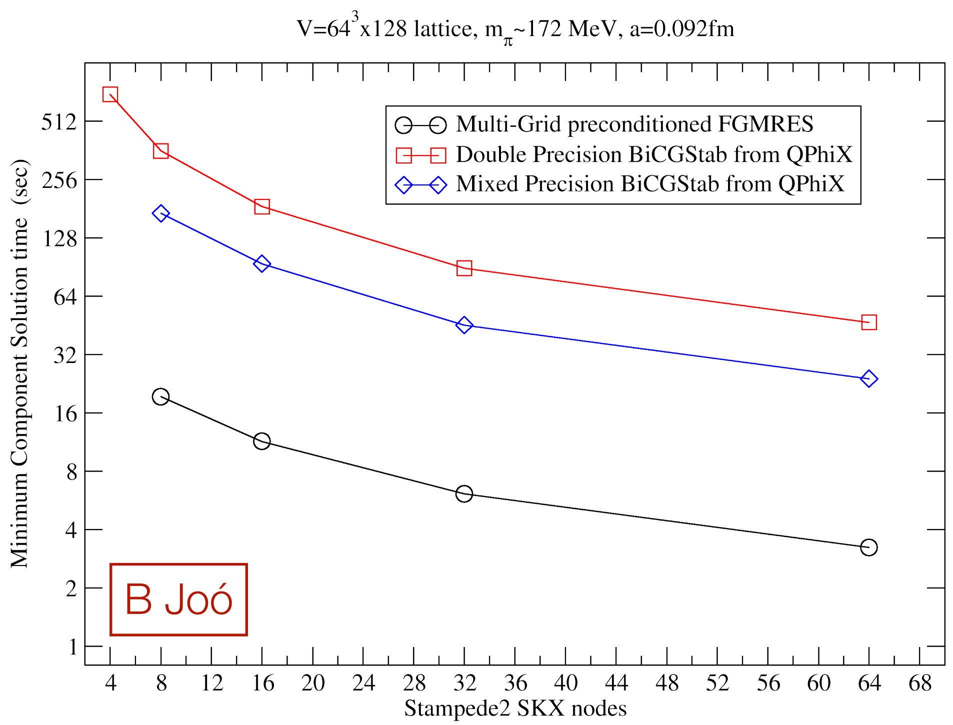
Critical collaboration with industry (NVIDIA)

summit

Computational advances

Iterative solvers





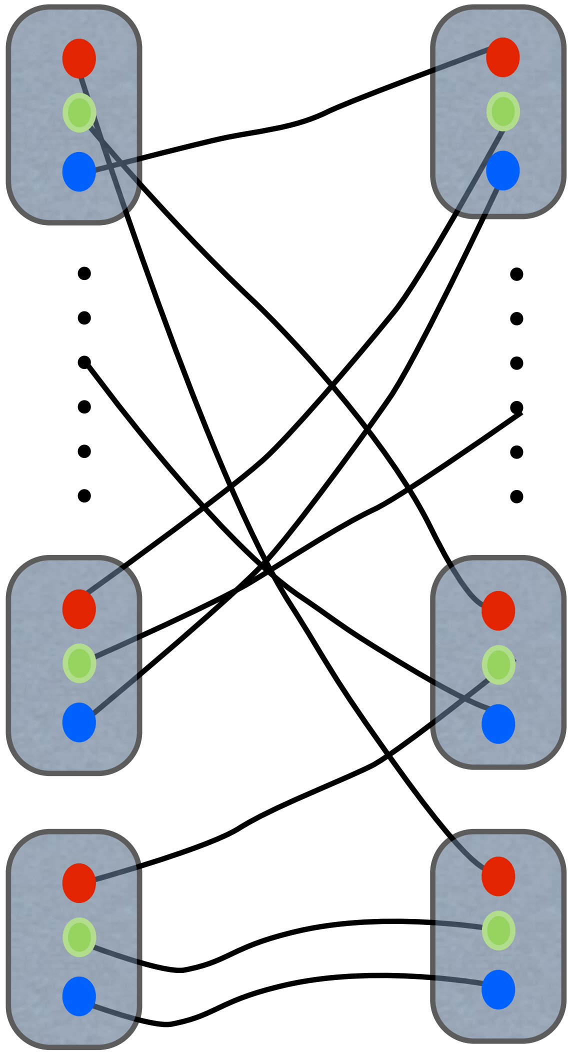
- Making use of new machines requires porting exisiting codes
- Architectural constraints preference different algorithms
  - Eg: GPUs favour communication-avoiding algorithms

Porting existing codes to new architectures requires significant investment

Computational advances

Contraction costs

- Contraction of quark fields scales factorially in system size/complexity
  - Grow to be comparable to gauge generation and inversions
- Graph methods to remove redundant work, code generators to optimise execution
- MIT (physics + CS): tiramisu code generator speeds up baryon-baryon contractions by 90x
- JLab: 8x MI-100 AMD GPU node is 400x performance of KNL node for 20x the cost



Productive collaborations with CS & Applied Maths

Computational advances

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Perlmutter, Frontier & Aurora exascale readiness
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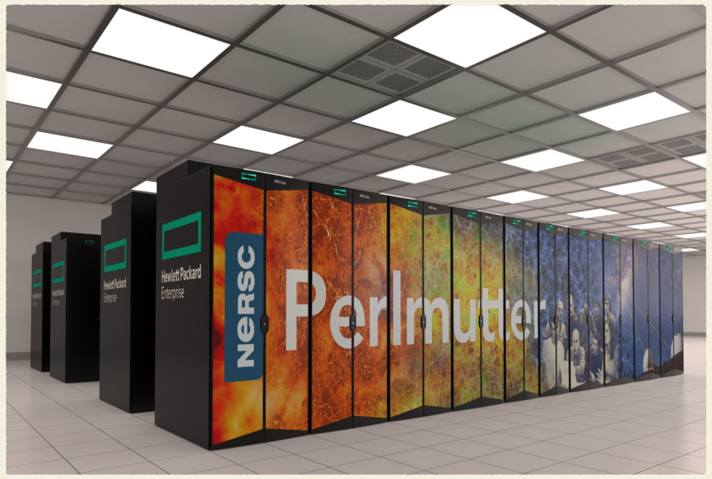


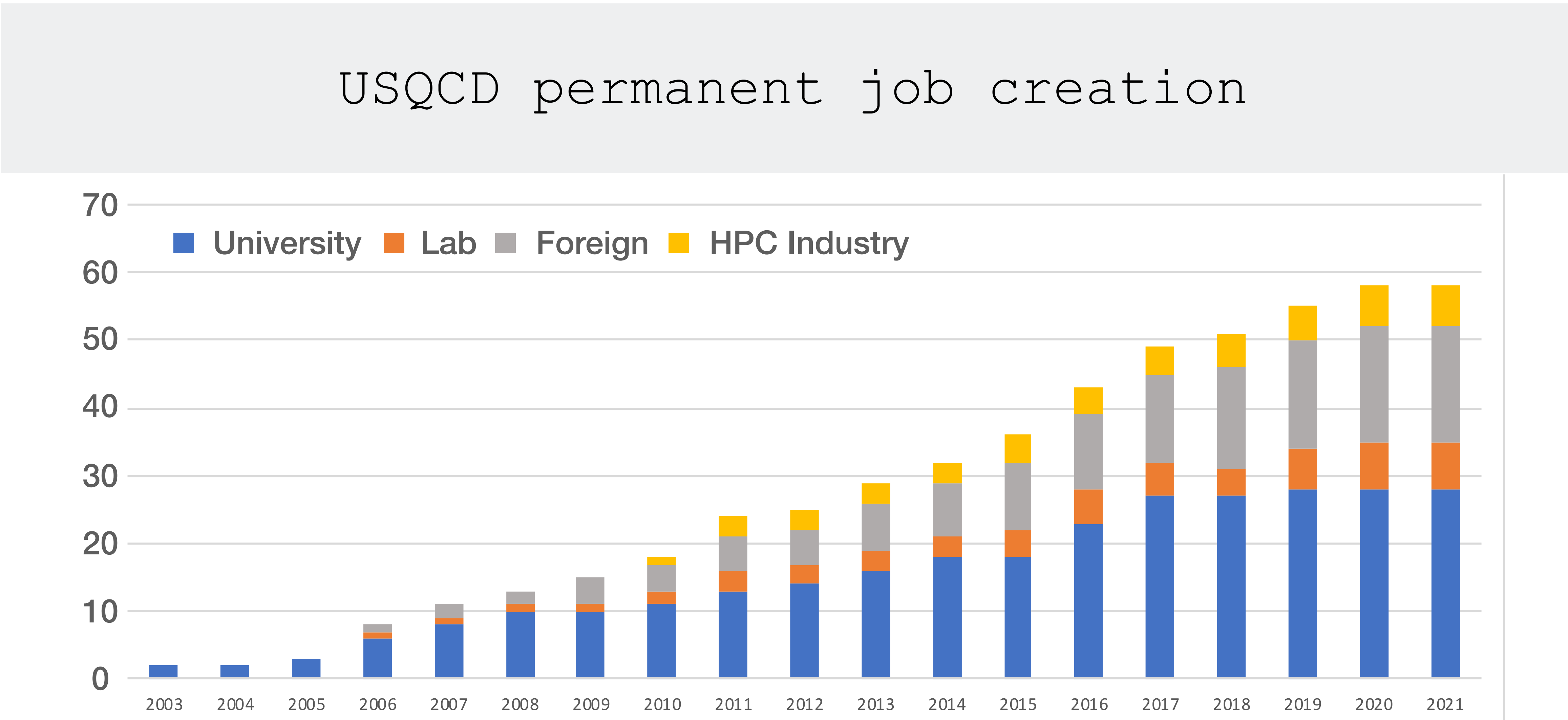
- LQCD is ready to run on all 3 (pre-)exascale architectures
  - Large-scale sustained effort from USQCD under SciDAC & ECP
  - Critical collaborations with industry partners and computing facilities
  - LQCD facilities provide hardware testbeds for application development

Computational advances

`AI/ML and quantum computing: future promise`

- New developments in AI/ML are leading to innovations in LQCD
  - Flow models for gauge generation: promise to overcome critical slowing down as continuum limit is taken (now for full QCD)
  - New ways to define observables with better statistical properties
  - Address the difficult inverse problems that arise in any areas: PDF fitting, hot QCD spectral functions…
- Quantum computing has promise to address questions that are beyond the capabilities of classical hardware (exascale and beyond)
  - Real time dynamics, nonzero baryon density,….

Workforce development & training

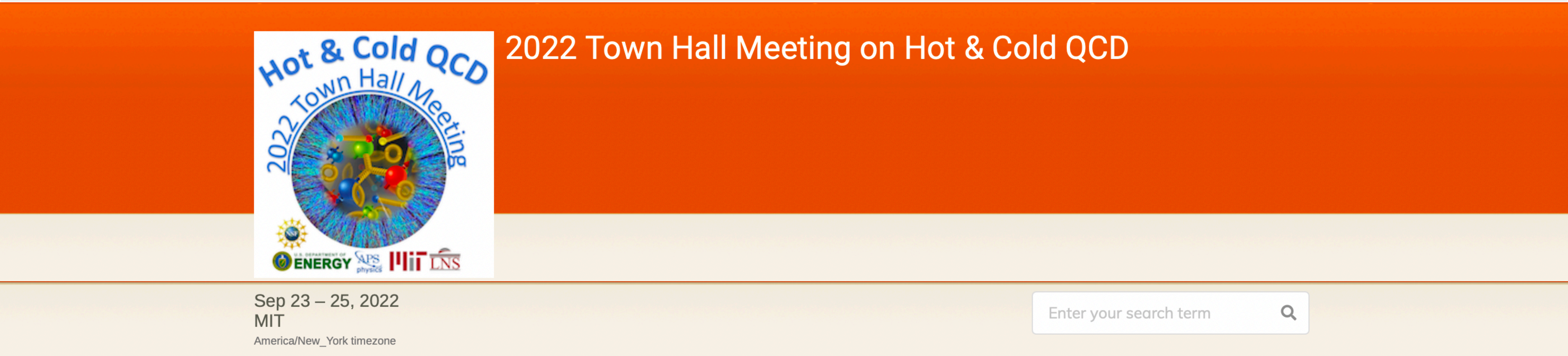


- USQCD faculty/lab job creation
- Strong (and rewarding!) pipeline to HPC industry (lower bound above)
- High demand for HPC expertise (>120 USQCD PhDs since 2000)

Workforce development & training

Summer schools and training programs

- Summer schools provide key training opportunity not available elsewhere
  - Frontiers of the field including ML and QC
  - Hands-on with code and algorithms
- Current proposal to DOE (MSU, MIT, UIUC, UConn, UMd, Colorado) for USQCD-based training project
  - Support beginning grad students with a lab-mentor program & dedicated courses
  - Broaden participation of underrepresented groups in LQCD/HPC



Computational QCD well-represented

- Organizing committee: Ian Cloet, Swagato Mukherjee
- Plenary speakers: Martha Constantinou, Phiala Shanahan
- Cold QCD parallel speakers: Yong Zhao, Xiangdong Ji
- Hot QCD parallel speakers: Peter Petreczky, Claudia Ratti, Abhijit Majumder