

# Jefferson Lab LQCD Computing

April 2021 All Hands Meeting

Robert Edwards

# Structure of NP/LQCD & JLab/LQCD programs

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- Organizational structure is that all computing at JLab is under (new) Computational Sciences & Technology Division (CST) with its own Assoc. Dir.
- JLab Theory group leader is “Assoc. Dir. for Computations and Nuclear Theory”
- LQCD@JLab started in ~FY01 - all funds directed through JLab/Theory
  - Theory and CST group have worked closely over 20 years
  - CST division very responsive to needs of LQCD Theory
- Systems deployed based on computational requirements for LQCD Theory program & serve LQCD community as a whole
  - Program is coordinated with USQCD and Scientific Program Committee
  - Funding directly from NP
- Similar structure for Experimental Nuclear Physics at JLab & computing
  - Expt. Physics Div. receives funds with computing systems operated by CST

# Nuclear and Particle Physics Computing Initiative

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NPPLCI started in 2018 - PI for project was Chip Watson, now Robert Edwards

- JLab - single purpose lab, NP funded, serves all of USQCD, and is complementary to the modified (2 lab, IC based) HEP LQCD project
- \$1M per year, about half hardware, half labor  
(equals average NP investment per year at JLab for last 10 years, so no real change in funding for the lab)
- FY2018: upgraded Jlab's KNL resources (added to system from FY2016)
- FY2019: upgraded Jlab's GPU resources (gamer-card system)
- FY2020/21: new AMD CPU + GPU system

More details in talks by Bryan Hess and Amitoj Singh

# Nuclear and Particle Physics Computing Initiative

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- Going forward, DOE asked JLab to merge LQCD into JLab Theory Group Annual reporting structure
  - First report (in Feb. 2020) included highlights of scientific program and future plans
  - Expect to carry this structure going forward
- DOE responds to the reports; however, not under an annual panel review process
- Instead, anticipate a broad review at the 4-year NP Theory Comparative reviews
  - Version in 2013 was across all of NP Theory (labs + universities)
  - 2016 review was only lab programs
  - Expect soon (2021?) at least a review of lab theory programs

# JLab & software development

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- Heavy involvement since 2001 & SciDAC-1, then SciDAC-2 & 3
- Currently, lead institution for ASCR/NP SciDAC-4 project
  - involving MIT, BNL, ORNL, W&M, GWU, MSU, UNC, LANL + industry
- Also direct NP portion under Exascale Computing Project
  
- Programs allow LQCD to leverage our local/commodity resources into efficiently utilizing national resources
  - This is how LQCD & NP in particular got onto ORNL NVIDIA systems early on
  - But these days, GPU-s are the main game in town
  
- Frontier+Aurora have pushed the “s” in GPU-“s”
  - Opportunity/necessity to diversify our codes
- Opportunity for LQCD to exploit for new commodity-based systems

# Exascale Computing Project

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- At some point, became clear
  - [Not Exascale] [Perlmutter](#) - AMD CPU + NVIDIA GPU + Cray network - now
  - [Frontier](#) - AMD CPU + AMD GPU + Cray network - soon
  - [Aurora](#) - Intel CPU + Intel GPU + Cray network - not as soon
- Thrusts for code bases
  - NVIDIA widely supported - new activities devoted to “refactorizing”
  - QUDA refactorized - now “backend” support for NVIDIA+AMD+Intel GPUs
  - Grid support for all, but focused more on Intel
  - CPS & MILC - rely on QUDA, but more focused towards Intel
  - **NDA-s huge restriction - limit informed public discussions**
- NP & Chroma - refactored to support more GPU systems, but prioritized AMD
  - **Support now for AMD+NVIDIA quite mature - some parts production ready**
  - **Software available on GitHub**

# New LQCD system acquisitions

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- JLab carried out an “Alternatives Analysis” and finished in early 2020
  - Gamer GPU system served limited set of applications
  - Input from community - need to expand portfolio of applications
  - AMD GPU an emerging technology in addition to NVIDIA
  - Consider two main metrics to quantify price-performance
    - Wilson dslash - proxy for inverters
    - ZGEMM based contractions considering possible swapping to main memory
- Development under ECP & SciDAC allowed for benchmarks across different systems
- Selected an AMD based system

See more details in talk by Amitoj Singh

<https://lqcd.jlab.org> - all project details, including usages here

The screenshot shows the Jefferson Lab LQCD web portal dashboard. The top navigation bar includes 'Getting Started', 'Support', and 'Staff Members'. The left sidebar contains menu items: Cluster Info (Nodes, Jobs, Usages), File System (Lustre, Cache, Volatile, Work), Tape Library, System, Documentation, and Administration. The main content area is titled 'Jefferson Lab LQCD' and contains a welcome message, two news items, and several performance metrics.

### Jefferson Lab LQCD

Welcome to the Jefferson Lab Lattice QCD computing home page. [New users start here.](#)

**Apr-21-21** **New lqcd web portal online** Please change the lqcd web portal bookmark to <https://lqcd.jlab.org>. The new web application, which utilizes Angular opensource web application framework, aims to provide more system status and statistical information to users and projects in addition to offer better user web experience. Please send suggestions and requests to [scicompdev@jlab.org](mailto:scicompdev@jlab.org).

**Apr-16-21** **Tape offline issue** In the last a few months, there were a few tapes damaged due to isolated LTO8 tape drive problems which has been diagnosed and fixed by IBM. Those tapes were sent back to IBM for data recovery. If a user failed to run srmGet to retrieve the files from tape library, executing **srmRequest id** will return messages like **request id: failed (Tape (xxxxx) is disabled for stub file (/mss/lattice/....** A request will fail if any of the file in the request is on offline tape. User can use [this page](#) to find out which files are currently on the offline tapes.

#### Phi Cluster (Slurm)

89%	90%	89%
Total	18p	16p
444	180	264

#### 19g Cluster

100%	100%
Total	19g
32	32

#### File System

lustre	/cache	/volatile	/work	/home
62%	99%	61%	58%	38%

#### Slurm Outstanding jobs

Running	Pending	Held	Other
239	9015	0	4

#### Slurm past 24 Hrs finished jobs

Success	Failed	Cancelled	Timedout	OverMemeory
5685	79	170	3	0

Last updated: Fri Apr 30 2021 02:29:46 GMT-0400 (EDT)



# Next up is JLab LQCD operations

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- Organizational structure:
  - Computational Sciences & Technology
    - Graham Heyes - Head of Scientific Computing - overseas operations of LQCD
    - Amitoj Singh - LQCD Site Manager - in April assumed position from Bryan Hess
    - Jie Chen - Performant Cluster Scientific Computing Group Leader (PCSCI)
    - Frank Winter - PCSCI
    - Eloy Romero - PCSCI
  - Theory
    - Robert Edwards - NP initiative manager & Deputy Theory Group Leader
- Presentations by Bryan Hess (operations) & Amitoj Singh (new purchases)