SciDAC-4 LQCD project kick-off meeting at TJLab
January 8-9, 2018

Based on slides from Robert Edwards' talk at the meeting

SciDAC-4

- Welcome to our new project:

  - "Computing the Properties of Matter with Leadership Computing Resources"

    - Lead PI: Robert Edwards (TJLAB)

    - Co-PIs: Will Detmold (MIT), Balint Joo (JLab), Swagato Mukherjee (BNL)

    - Sept. 2017 - Sept. 2022: $4M NP (Ted Barnes) & $4.25M ASCR (Randall Laviolette)

    - Originally requested $10M: some trimming, reduced overhead, removed some PD years

  - Senior Investigators:

    - Andrei Alexandru (GWU/Physics), Saman Amarasinghe (MIT/CS), Alexei Bazavov (MSU/Physcs), Kate Clark (NVIDIA), Rob Fowler (UNC/RENCI), Xu Liu (W&M/CS), Kostas Orginos (W&M/Physics), Sergey Panitkin (BNL/Physics), Andrew Pochinsky (MIT/Physics), Kenny Roche (PNNL/UW/Physics), Martin Savage (UW/INT), Frank Winter (JLab), Boram Yoon (LANL/CS)

Publicity and useful repositories

GitHub: https://github.com/LQCDSciDAC4   Website: https://lqcdscidac4.github.io

Organized around science   goals

Science areas recognized in the 2015 NSAC Long Range Plan

- Extreme matter at high temperatures and/or densities
  - BNL and a future EIC
  - DOE Topical collab. (Mukherjee)
- Hadron spectroscopy
  - CLAS12 & GlueX @ JLab
- Hadron structure
  - JLab, RHIC-Spin @ BNL, future EIC
  - DOE Topical collab. (J.W. Qiu & W. Detmold)
- Nuclear structure and interactions
  - soon FRIB, components of SM tests at JLab
- Tests of fundamental symmetries
  - Violations of SM, parity violating expts, proposed new low-energy facilities

SciDAC: organize around sites and themes

- JLab (Joo):
  - Clover gauge generation central to T=0 NP program
    - New algorithms efforts (1-flavor, gauge integration, new solvers) + LCF readiness
    - Code optimizations
  - Support for hadron structure efforts
  - Collaborations with LANL, W&M, GWU, UNC

- MIT (Detmold)
  - Analysis: many-body correlation functions
  - Optimal code generation
  - Collaborations with PNNL/UW

- BNL (Mukherjee)
  - HISQ finite T and also anisotropic HISQ for heavy flavor physics at finite T
  - Workflow of jobs: support for large valence analysis campaigns
  - Collaborations with MSU

Resources

- Allocations today
  - USQCD:
    - INCITE: Titan (OLCF): 100M core-hours (~3M K20 GPU-hours)
    - INCITE: Mira (ALCF): 300M BGQ core-hours (~18M node-hours)
    - Dedicated: ~4M K20 GPU-hours + 3M KNL node-hours + 0.5M Skylake node-hrs (BNL)
  - INCITE (Orginos): 100M (Titan) + ?? (Mira)
  - NERSC: Cori: ~ 300M (?) available for all of NP (e.g., lqcd, astro, etc.)
  - NCSA: Bluewaters: no NP allocation. Bids out for new NSF system
- SummitDev (OLCF)
  - Been available for testing - Power8+Pascal. Suppose to become allocated
- Summit:
  - Coming on-line now (2018). ~4600 nodes of 2*Power9+6*Volta
  - First ESP allocations. Then regular INCITE/ALCC in Jan 2019
  - USQCD/NP/T=0 (PI: Edwards) and T!=0 (PI: Mukherjee) each submitted a LOI
    - Allows for testing on full system
  - ESP proposals due by June
- NERSC9: CY20

Relation to Exascale Computing Project (ECP)

- Scope of ECP:

    - Focused on longer term: originally Exascale in ~CY24 (accelerated to CY21)

    - Overarching goal: large physical volumes, small lattice spacings, complicated observables at Exascale

    - Centered on 4 themes:

        - Software API-s/implementations (Carleton DeTar)

        - Dirac solvers (Richard Brower)

        - Critical slowing down in gauge generation (Norman Christ)

        - Evaluating many-body correlation functions (Edwards)

    - Milestones & deliverables associated with each

Pre-exascale system plans (*now   out-ofdate*)
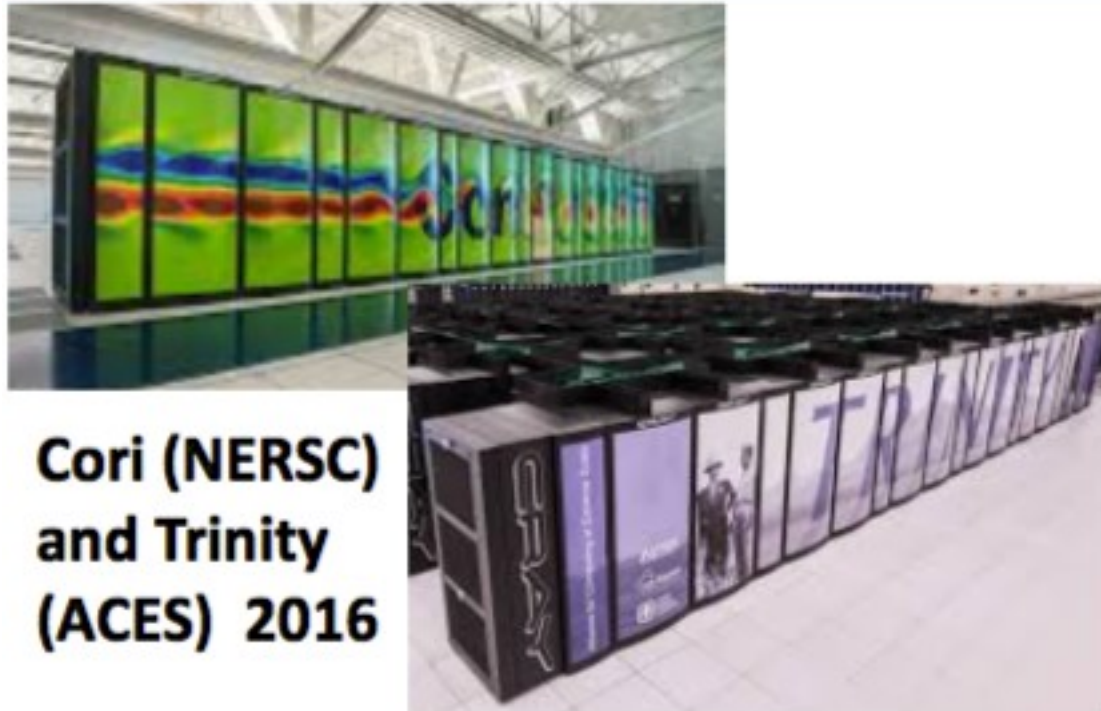

Theta (ALCF) 2016

Summit (OLCF) and
Sierra (LLNL), 2018
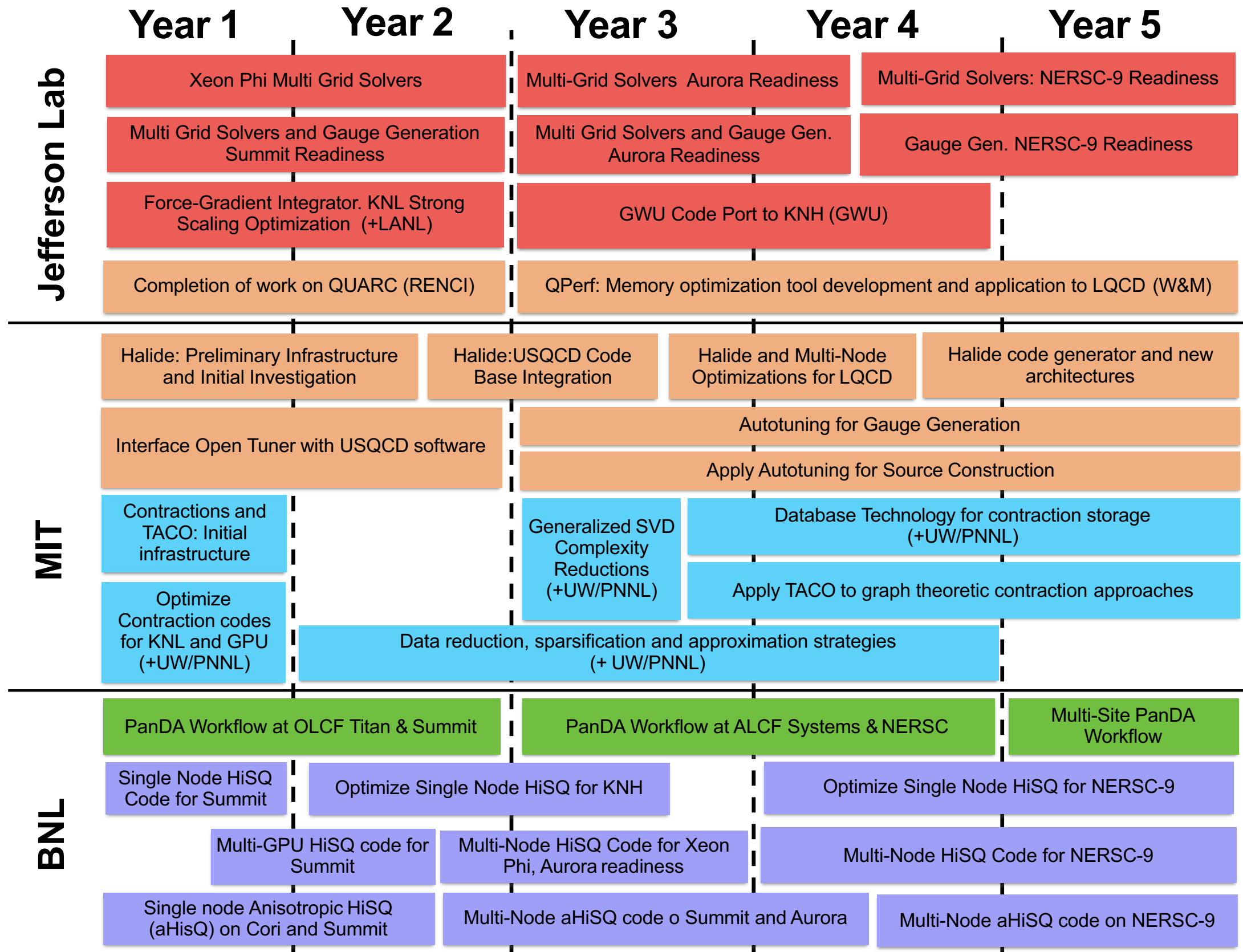
Crossroads (ACES)
and NERSC-9, 2020

2016   2018   2020

Cori (NERSC)
and Trinity
(ACES) 2016

Aurora: now 2021

Proposed work plan

	Year 1	Year 2	Year 3	Year 4	Year 5

Jefferson Lab

- Xeon Phi Multi Grid Solvers
- Multi-Grid Solvers Aurora Readiness
- Multi-Grid Solvers: NERSC-9 Readiness
- Multi Grid Solvers and Gauge Generation Summit Readiness
- Multi Grid Solvers and Gauge Gen. Aurora Readiness
- Gauge Gen. NERSC-9 Readiness
- Force-Gradient Integrator. KNL Strong Scaling Optimization (+LANL)
- GWU Code Port to KNH (GWU)
- Completion of work on QUARC (RENCI)
- QPerf: Memory optimization tool development and application to LQCD (W&M)

MIT

- Halide: Preliminary Infrastructure and Initial Investigation
- Halide:USQCD Code Base Integration
- Halide and Multi-Node Optimizations for LQCD
- Halide code generator and new architectures
- Interface Open Tuner with USQCD software
- Autotuning for Gauge Generation
- Apply Autotuning for Source Construction
- Contractions and TACO: Initial infrastructure
- Generalized SVD Complexity Reductions (+UW/PNNL)
- Database Technology for contraction storage (+UW/PNNL)
- Apply TACO to graph theoretic contraction approaches
- Optimize Contraction codes for KNL and GPU (+UW/PNNL)
- Data reduction, sparsification and approximation strategies (+ UW/PNNL)

BNL

- PanDA Workflow at OLCF Titan & Summit
- PanDA Workflow at ALCF Systems & NERSC
- Multi-Site PanDA Workflow
- Single Node HiSQ Code for Summit
- Optimize Single Node HiSQ for KNH
- Optimize Single Node HiSQ for NERSC-9
- Multi-GPU HiSQ code for Summit
- Multi-Node HiSQ Code for Xeon Phi, Aurora readiness
- Multi-Node HiSQ Code for NERSC-9
- Single node Anisotropic HiSQ (aHisQ) on Cori and Summit
- Multi-Node aHiSQ code o Summit and Aurora
- Multi-Node aHiSQ code on NERSC-9

Summary

- High visibility project with multiple important science drivers
- Supported for 5 years by DOE NP and ASCR (SciDAC-4)
- Strong connection to DOE supported physics programs and experimental facilities
- The project is computationally intensive, with large allocations on multiple sites (ALCF, NERSC, OLCF; LQCD clusters at BNL, FNAL and TJLAB,…)
- Natural interest in campaign style job submissions to multiple HPC sites
- The project has software development and WMS components
    - PanDA is WMS of choice
- Emerging collaboration between BNL and TJLab (Edwards, Trewartha) in WMS domain
- First meeting on Jan 16, 2018 to discuss cooperation and possible first steps
    - PanDA edge services install at TJLab on LQCD cluster and/or Titan by Daniel Trewartha using PanDA tools and documentation
    - Development of tools to run several types of LQCD workloads and enable production campaigns O(100k jobs)
    - Improve understanding of LQCD workflows
    - Understand data management requirements for LQCD especially for multi-site operations