# Report on QCDOC at BNL

All Hands' Meeting US Lattice QCD Collaboration Meeting FNAL, April 6-7, 2006

> Stratos Efstathiadis BNL



#### OUTLINE

#### • Introduction

QCDOC Overview

(Architecture, Available Partitions, Current Status)

• User Environment and Monitoring

(Network, Batch System, Resource Monitoring...)

Conclusions



#### Introduction

- QCDOC: Quantum ChromoDynamics On Chip
- Optimized for Lattice QCD Calculations Capable of <u>strong scaling</u>: use many nodes on a small problem:
  - Large inter-node bandwidth
  - Small communications latency
- Designed for optimal price/performance, low power, modular design, high scalability and reliability.
- Collaboration between IBM, Columbia, UKQCD, RBRC and BNL
- Three large QCDOC machines in production.



# **QCDOC** Collaboration

- Columbia (DOE)
  - Norman Christ
  - Saul Cohen
  - Calin Cristian
  - Zhihua Dong
  - Changhoan Kim
  - Ludmila Levkova
  - Xiaodong Liao
  - Meifeng Lin
  - Guofeng Liu
  - Robert Mawhinney
  - Shu Li
  - Azusa Yamaguchi
- BNL (SciDAC)
  - Chulwoo Jung
  - Konstantin Petrov
  - Stratos Efstathiadis

Brookhaven Science Associates U.S. Department of Energy

- UKQCD (PPARC)
  - Peter Boyle
  - Mike Clark
  - Balint Joo

#### • RBRC

- Shigemi Ohta
- Tilo Wettig

#### • IBM

- Dong Chen
- Alan Gara
- Design groups:
  - Yorktown Heights, NY
  - Rochester, MN
  - Raleigh, NC



# **QCDOC** Chip





#### **QCDOC** Construction



An ASIC (node). ~5 Watt at 400MHz



A daughterboard with two nodes and the vertically mounted DDR SDRAMs (128MB at BNL)



A single motherboard. Two rows of 16 daughterboard with 2 nodes each provide a total of 64 nodes. 14.5in x 27 in



A water-cooled rack containing 16 MBds with 1024 nodes. The upper compartment holds Ethernet switches

#### MACHINE OVERVIEW

Networks:

- Black squares are nodes
- Blue Boxes are Mother boards
- Red Lines are communication links
- Green lines are Ethernet connections
- Green boxes are Ethernet switches
- Pink boxes are host CPU processors





RBRC (right) and DOE (left) 12K-node QCDOC machines

USDOE QCDOC Dedication Ceremony November 30<sup>th</sup> 2005.





# Current QCDOC Usage

	Machine partition	Nodes	Wired	Use
MILC (Dru Renner, Carleton Detar)	Rack 24-27	4096	8x8x8x2x2x2	48^3 x 144 lattice generation
	Rack 22-23	2048	16x4x4x2x2x2	40^3x96 lattice generation
RBC (Norman Christ, MF Lin, S.Cohen)	Rack 20-21	2048	16x4x4x2x2x2	DWF
LHPC (R. Edwards)	Rack 19	1024	8x4x4x2x2x2	Hadron Structure on MILC Lattices
Thermodynamics (Karsch Frithjof, Chulwoo Jung)	Rack 18	1024	8x4x4x2x2x2	P4 Thermodynamics
	Rack 17 – crate1	512	4x4x4x2x2x2	
	Rack 17 – crate 0	512	4x4x4x2x2x2	
LHPC (Dru Renner)	Rack 16 (14 MBs)	896	14x4x2x2x2x2	DWF Propagator Generator
	Rack 16 – crate 0 – slot 0	64		
	Rack 16 – crate 1 – slot 0	64		

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U.S. Department of Energy



#### The QCDOC Network Enclave



#### The QCDOC Network Enclave



#### Host Computer

- The front-end host is an IBM P655 server with 8CPUs, 8GB of memory running AIX.
- Multiple network interfaces provide access to machine partitions.
- Users cross-compile code and manage allocated machine partitions using host software (qdaemon, qcsh).



#### Disk Systems: /host

• A custom NFS client is part of the node kernel supporting two mount points (open/read/write/close).

• A disk file system that is globally shared by all partition nodes and accessible by the front-end system.

• Usually a disk on the front-end systems.



#### Disk Systems: /pfs

• The Parallel File System (pfs) is used for high throughput IO from machine partition nodes.

•Provided by 2U rack-mounted LINUX NAS Servers. 2 RAID-5 file servers per machine rack (one per crate), total disk space 48TB.

- Similar to cluster "scratch-disk" on every node.
- Each NAS is shared by several nodes. Each node is using a unique directory, ex. /R24/C0/B0/D21/A1/
- Temporary data staging, not backed up.
- Accessible by the front-end systems (ex. /pfs/r16c0/R16/C0/...)
- Tunned NFS, RAID controller and kernel parameters to optimize IO performance (same I/O tunning across the Atlantic).

Local Storage and transfers of Lattice Configurations

• 10 4.8TB ANACAPA file servers make up five archive/backup pairs. The five archive servers are automounted on the front-end host while the backup servers simply mirror the archives.

• Transferring files to BNL (or Jlab) may be a 2-hop process or use ssh tunneling (dedicated qcdoc ssh gateways at BNL).

• Transferring files to FNAL, a kerberized utility must be used (rcp, scp) after obtaining a kerberos ticket (kinit).



# Lattice Configurations on the web

• The purpose is to make a number of generated lattices easily available to the community with various degrees of password protection.

•Set up web site inside qcdoc network enclave (reverseproxy to the outside world): http://qcdlattices.bnl.gov

• Configurations can be downloaded via http. Provide tools to easily download "clusters" of lattices (wget wrapper).

• Configurations are in the QCD Archive Format.



#### Resource Monitoring (Servers)

• Nagios monitors our servers (front-end, archive, pfs, host and home file servers and ssh gateways) for usage CPU loads, services (ssh, NFS), disk space etc.

QCDOC Systems - high priority (gcd-important)

Host	Services
<u>qcdochosta.qcdoc.bnl.gov</u>	DISK:/ DISK:/data0_DISK:/host_DISK:/host-r12_DISK:/host1_DISK:/opt_DISK:/pfs/acc5_DISK:/pfs/acc8 DISK:/pfs/r04_DISK:/pfs/r05_DISK:/pfs/r06_DISK:/pfs/r07_DISK:/pfs/r08_DISK:/pfs/r09_DISK:/pfs/r10_DISK:/pfs/r DISK:/pfs/r12_DISK:/pfs/r13_DISK:/pfs/r14_DISK:/pfs/r15_DISK:/qcdoc_DISK:/qdata00_DISK:/space_DISK:/tmp DISK:/usr_DISK:/var_LOAD_NES_server:10.20.1.10_NES_server:pfs-acc5_NES_server:pfs-acc8_NES_server:pfs-r0 NES_server:pfs-r06_NES_server:pfs-r07_NES_server:pfs-r08_NES_server:pfs-r09_NES_server:pfs-r10_NES_server:p r12_NES_server:pfs-r13 NES_server:pfs-r14_NES_server:pfs-r15_NES_server:qcdraida_NES_server:qcdraidb_SSH
gcdochostb.qcdoc.bnl.gov	DISK/ DISK/rarchive/a0_DISK./archive/a1_DISK/rarchive/a2_DISK/rarchive/a3_DISK/rarchive/a4_DISK/host_DISK DISK/host-r18c0_DISK/host-r19c0_DISK/host-r20c0_DISK/host-r22-23_DISK/host-r24-27_DISK/host_DISK/ DISK/pfs/r16c0_DISK/pfs/r16c0a_DISK/pfs/r16c1_DISK/pfs/r16c1a_DISK/pfs/r17c0_DISK/pfs/r17c1_DISK/pfs/ DISK/pfs/r19c0_DISK/pfs/r19c1_DISK/pfs/r20c0_DISK/pfs/r20c1_DISK/pfs/r21c0_DISK/pfs/r21c1_DISK/pfs/ DISK/pfs/r23c0_DISK/pfs/r23c1_DISK/pfs/r24c0_DISK/pfs/r24c1_DISK/pfs/r25c0_DISK/pfs/r25c1_DISK/pfs/ DISK/pfs/r27c0_DISK/pfs/r21c1_DISK/pfs/r24c0_DISK/rfs/r24c1_DISK/yfs/r25c0_DISK/pfs/r25c1_DISK/pfs/ DISK/pfs/r27c0_DISK/pfs/r21c1_DISK/pfs/r24c0_DISK/rfs/r24c1_DISK/war_LOAD_NES_server.doearchive0 NES_server.doearchive1_NES_server.pfs-r16c1_NES_server.pfs-r16c0_ NES_server.pfs-r16c0a_NES_server.pfs-r16c1_NES_server.pfs-r16c1a_NES_server.pfs-r17c0_NES_server.pfs-r17c1_ r18c0_NES_server.pfs-r18c1_NES_server.pfs-r19c0_ NES_server.pfs-r19c1_NES_server.pfs-r20c0_NES_server.pfs-r20c1_NES_server.pfs-r21c0_NES_server.pfs-r21c1_I r22c0_NES_server.pfs-r23c1_NES_server.pfs-r23c0_ NES_server.pfs-r23
gcdraida.gcdoc.bnl.gov – 🌇	DISK:/ DISK:/boot LOAD SSH
acdraidb.acdoc.bnl.aov 🛛 🕵	DISK:/ DISK:/boot LOAD SSH

# **QCDOC Batch System**

- Goal: increase machine usage and productivity.
- Standard Batch features:
  - File Staging
  - Accounting
  - Job Status Notification
  - ACLs
  - Resource Limits
- Added Features in scripts:
  - Partition Allocation
  - Partition Startup
  - Idle Job checks
  - Partition resets and Powercycling
  - qhdwcheck wrapper
  - Job re-runs and Error Limits
  - Error and Event Logging, User Notification

### **QCDOC Batch System**

- PBS (Torque) with MAUI scheduler.
- •Restricted machine partitions:
  - Each mapped to a PBS queue.
  - Simple FIFO scheduling
  - ACL limits user access
  - No limits on resource usage
  - Partition can allocated using the web allocator
- ACC Single MBd partitions:
  - Queues with walltime limits (<u>OneHr</u>, <u>FourHr</u>, <u>EightHr</u> and <u>SixteenHr</u>) on four MBds (slot4-7)
  - Queued jobs may transfer to empty (not running) queues.
  - Queues can be marked as unavailable if there are hardware problems
- Latest version of PBS scripts: /qcdoc/local/batch/v3
- Web site: http://www3.bnl.gov/qcdoc/pbs

#### Job Accounting

Monitor <u>qdaemon</u> and <u>qcsh</u> processes on the front-end host: http://www3.bnl.gov/qcdoc/status

#### **QCDOC Current Status**

(Water-Cooled Racks Only)

Partition (Click for partition details)	Allocated? (Click to Allocate)	Alloc. User	Run User (Click for User Jobs)	Run Time [Days-]Hrs:Mins:Secs		
rack16/14mb	True	drenner	drenner	3-12:28:58		
rack16/crate0/slot0	False	-	-	-		
rack16/crate1/slot0	True	mawhinne	-	-		
rack17/crate0	True	chulwoo	<u>chulwoo</u>	08:44:50		
rack17/crate1	True	chulwoo	<u>chulwoo</u>	9-15:30:48		
rack18	True	chulwoo	<u>chulwoo</u>	06:50:32		
rack19	True	edwardsr	edwardsr	2-09:15:12		
rack20-21	True	sdcohen	sdcohen	4-01:11:23		
rack22-23	True	drenner	drenner	3-17:52:12		
rack24-27	True	drenner	drenner	17:33:02		
Current Status List All Running List All Done List All Jobs						

# Error Accounting and Daughterboard Tracking

- QOS reports:
  - List of daughterboards in machine partition (location files).
  - List of generated errors (Dbd, Wire and Ethernet).
- *qhdwcheck* wrapper stores error counters in a database.
- User reported problems via CTS.
- Web Fronts (jsp) by Joe Aronson (SUNY SB): http://www3.bnl.gov/qcdoc/errors

#### QCDOC Hardware Monitoring (Safety System)



1. DELTA DEW POINT IS CHWS TEMP MINUS DEW POINT IF 0 OR NEGATIVE SWEATING OCCURS



## Summary/Future Plans

- The USDOE QCDOC machine at BNL is in full production.
- Largest partition is a 4-rack machine (4096-node).
- Half of the machine (6 racks) is used by MILC producing lattice configurations at a steady rate.
- All partition nodes are running at 400MHz
- Hardware issues:
  - Lost Ethernet Contact (infreq. during booting or I/O). May recover with a software reset or may require power cycle.
  - Serial Communication Errors
- Improve our (common) runtime environment
- *qrun* wrapper
- Interactive PBS queues.
- Improve and use hardware error tracking

#### Conclusions

- QCDOC Web Site at BNL: http://www.bnl.gov/lqcd/
- Web Allocator: https://rbc.bnl.gov/
- Call Tracking System (CTS): https://qcdoc.phys.columbia.edu/cts
- Batch system: http://www3.bnl.gov/qcdoc/batch/pbs
- QCDOC people at BNL (Led by Bob Mawhinney)

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