

Blue Gene/Q and Knights Landing Many Core Architectures Argonne Training Program on Extreme Scale Computing

Scott Parker Argonne Leadership Computing Facility 8/01/2016





Argonne HPC Timeline

2004:

- Blue Gene/L introduced
- LLNL 90-600 TF system #1 on Top 500 for 3.5 years
- **2005**:
 - Argonne accepts 1 rack (1024 nodes) of Blue Gene/L (5.6 TF)
- **2006**:
 - Argonne Leadership Computing Facility (ALCF) created
 - ANL working with IBM on next generation Blue Gene
- **2008**:
 - ALCF accepts 40 racks (160k cores) of Blue Gene/P (557 TF)
- **2009**:
 - ALCF approved for 10 petaflop system to be delivered in 2012
 - ANL working with IBM on next generation Blue Gene
- **2012**:
 - 48 racks of Mira Blue Gene/Q (10 PF) in production at ALCF
- **2014**:
 - ALCF CORAL contract awarded to Intel/Cray
 - Development partnership for Theta and Aurora begins
- **2016**:
 - ALCF accepts Theta (8.5 PF) Cray XC40 with Xeon Phi (KNL)
- **2018**:
 - Aurora (180+ PF) Cray/Intel Xeon Phi (KNH) to be delivered







Current ALCF Systems

Mira – BG/Q system

- 49,152 nodes / 786,432 cores
- 768 TB of memory
- Peak flop rate: 10 PF
- Linpack flop rate: 8.1 PF (#6 Top 500)

Cetus & Vesta (T&D) - BG/Q systems

- 4K & 2k nodes / 64k & 32k cores
- 64 TB & 32 TB of memory
- 820 TF & 410 TF peak flop rate

Cooley– x86 & Nvidia system

- 126 nodes / 1512x86 cores/ 126 nVidia Tesla K80 GPUs
- 47 TB x86 memory / 3 TB GPU memory
- Peak flop rate: 220 TF

Storage

Over 30 PB capacity, 240 GB/s bw (GPFS)



Blue Gene DNA And The Evolution of Many Core

Leadership computing power

- Leading architecture since introduction, #1 half Top500 lists over last 10 years
- On average over the last 12 years 3 of the top 10 machine on Top 500 have been Blue Genes
- Low speed, low power
 - Embedded PowerPC core with custom SIMD floating point extensions
 - Low frequency (L 700 MHz, P 850 MHz, Q 1.6 GHz)
- Massive parallelism:
 - Multi/Many core (L 2, P 4, Q 16)
 - Many aggregate cores (L 208k, P 288k, Q 1.5M)
- Fast communication network(s)
 - Low latency, high bandwidth, torus network (L & P 3D, Q 5D)
- Balance:
 - Processor, network, and memory speeds are well balanced
- Minimal system overhead
 - Simple lightweight OS (CNK) minimizes noise
- Standard Programming Models
 - Fortran, C, C++, & Python languages supported
 - Provides MPI, OpenMP, and Pthreads parallel programming models
- System on a Chip (SoC) & Custom designed Application Specific Integrated Circuit (ASIC)
 - All node components on one chip, except for memory
 - Reduces system complexity and power, improves price / performance
- High Reliability:
 - Sophisticated RAS (reliability, availability, and serviceability)
- Dense packaging
 - 1024 nodes per rack

BlueGene/Q Compute Chip



It's big

- 360 mm² Cu-45 technology (SOI)
- 1.5 B transistors
- 205 GF per node

18 Cores

- 16 compute cores
- 17th core for system functions (OS, RAS)
- plus 1 redundant processor
- L1 I/D cache = 16kB/16kB

Crossbar switch

- Each core connected to shared L2
- Aggregate read rate of 409.6 GB/s

Central shared L2 cache

- 32 MB eDRAM
- 16 slices

Dual memory controller

- 16 GB external DDR3 memory
- 42.6 GB/s bandwidth

On Chip Networking

- Router logic integrated into BQC chip
- DMA, collective operations
- 11 network ports

BG/Q Chip, Another View



BG/Q Core



- 2-way concurrent issue 1 XU + 1 AXU
- A given thread may only issue 1 instruction per cycle
- Two threads may simultaneously issue 1 instruction each cycle

QPX Overview

- Unique 4 wide double precision SIMD instructions extending standard PowerISA with:
 - Full set of arithmetic functions
 - Load/store instructions
 - Permute instructions to reorganize data
- 4 wide FMA instructions allow 8 flops/inst
- FPU operates on:
 - Standard scale PowerPC FP instructions
 - 4 wide SIMD instructions
 - 2 wide complex arithmetic SIMD arithmetic
- Standard 64 bit floating point registers are extended to 256 bits
- Attached to AXU port of A2 core
- A2 issues one instruction/cycle to AXU
- 6 stage pipeline
- Compiler can generate QPX instructions
- Intrinsic functions mapping to QPX instructions allow easy QPX programming



BG/Q Memory Hierarchy



The Blue Gene/Q Network

- 5D torus network:
 - Achieves high nearest neighbor bandwidth while increasing bisectional bandwidth and reducing hops vs 3D torus
 - Allows machine to be partitioned into independent sub machines
 - No impact from concurrently running codes.
 - Hardware assists for collective & barrier functions over COMM_WORLD and rectangular sub communicators
 - Half rack (midplane) is 4x4x4x4x2 torus (last dim always 2)
- Nodes have 10 links with 2 GB/s raw bandwidth each
 - Bi-directional: send + receive gives 4 GB/s
 - 90% of bandwidth (1.8 GB/s) available to user
- Hardware latency
 - ~40 ns per hop through network logic
 - Nearest: 80ns
 - Farthest: 3us (96-rack 20PF system, 31 hops)
- Network Performance
 - Nearest-neighbor: 98% of peak
 - Bisection: > 93% of peak
 - All-to-all: 97% of peak
 - Collective: FP reductions at 94.6% of peak
 - Allreduce hardware latency on 96k nodes ~ 6.5 us
 - Barrier hardware latency on 96k nodes ~ 6.3 us



Blue Gene/Q Software High-Level Goals & Philosophy

- Facilitate extreme scalability
 - Low noise on compute nodes
 - File I/O offloaded to I/O nodes running full Linux
 - GLIBC environment with a few restrictions for scaling
- Familiar programming modes such as MPI and OpenMP
 - Scalable MPICH2 providing MPI 2.2 with extreme message rate
 - Efficient intermediate (PAMI) and low-level (SPI) message libraries
 - PAMI layer allows easy porting of runtimes like GA/ARMCI, Berkeley UPC, etc
- Standards-based when possible
 - Linux development environment: familiar GNU toolchain with glibc, pthreads
 - XL Compilers C, C++, Fortran with OpenMP 3.1
 - Debuggers: Totalview
 - Tools: HPC Toolkit, TAU, PAPI, Valgrind
- Open source where possible
- Facilitate high performance for unique hardware:
 - Quad FPU, DMA unit, List-based prefetcher
 - TM (Transactional Memory), SE (Speculative Execution)
 - Wakeup-Unit, Scalable Atomic Operations
- Flexible and fast job control with high availability
 - Noise-free partitioned networks
 - Integrated HPC, HTC, MPMD, and sub-block jobs
- Facilitate new programming models

Future ALCF Systems

Theta

- Arriving in 2016
- Intel Xeon Phi, 2nd Generation (Knights Landing)
- 3,240 compute nodes: 207,360 cores
- 660 TB of memory
- 8.5 PetaFlops peak performance
- Cray Aries interconnect
- Dragonfly network topology
- 10 PB Lustre file system

Aurora

- Arriving in 2018
- Intel Xeon Phi, 3rd Generation (Knights Hill)
- Over 50,000 compute nodes
- Greater than 7 PB of persistent memory
- 180+ PetaFlops peak performance
- Intel Omni-Path interconnect
- Dragonfly network topology
- Over 150 PB Lustre file system



Knights Landing Processor



13

KNL Tile and Core



Tile

- Two CPUs
- 2 VPUs per core
- Shared 1 MB L2 cache (not global)
- Caching/Home agent
 - Distributed directory, Coherence

Core

- Based on Silvermont (Atom)
- Functional units:
 - 2 Integer ALUs
 - 2 Memory units
 - 2 VPU's with AVX-512
- Instruction Issue & Exec:
 - 2 wide decode
 - 6 wide execute
 - Out of order
- 4 Hardware threads per core



Programming with IPM and DRR



- Two memory types
 - In Package Memory (IPM)
 - 16 GB MCDRAM
 - ~480 GB/s bandwidth
 - Off Package Memory (DDR)
 - Up to 384 GB
 - ~90 GB/s bandwidth
- One address space
 - Possibly multiple NUMA domains
- Memory configurations
 - Cached: DDR fully cached by IPM
 - Direct mapped: user managed
 - Hybrid: ¼, ½ IPM used as cache
- Managing memory:
 - jemalloc &numa libraries
 - Pragmas for static memory allocations

Clustering Modes

Quadrant Mode





- 1. Tile has Cache Miss
- 2. CHA selected
- 3. Memory Controller
- 4. Memory Received

Aries Dragonfly Network



16 Aries routers

connected by

chassis backplane

4 nodes

connected to

each Aries

router

Aries Router:

- 4 NIC's connected via PCIe
- 40 Network tiles/links
- 4.7-5.25 GB/s/dir per link

Dragonfly topology

- 4 nodes connected to an Aries
- 2 Local all-to-all dimensions
 - 16 all-to-all horizontal
 - 6 all-to-all vertical
- 384 nodes in local group
- All-to-all connections between groups

Considerations In Moving From BG/Q to Xeon Phi (KNL)

More local parallelism

- 64-72 cores (KNL) vs 16 (BG/Q)
- 4 hardware threads on both

No increase in the number of nodes

Increased vector length

8 wide vectors (KNL) vs 4 wide vectors (BG/Q)

Increased node performance

- 2.4 TF (KNL) vs 0.2 TF (BG/Q)

Instruction issue

- Out-of-order (KNL) vs in-order (BG/Q)
- 2 wide instruction issue on both
- 2 floating point instructions per cycle (KNL) vs 1 per cycle (BG/Q)

Memory Hierarchy

MCDRAM & DDR (KNL) vs uniform 16 GB DDR (BG/Q)

Different network topology

- 5D torus vs Dragonfly
- NIC connectivity
 - PCIe (Aries, Omni-Path) vs direct crossbar connection (BG/Q)

Questions?