Gateways to Discovery: Cyberinfrastructure for the Long Tail of Science

ECSS Symposium, 12/16/14

HPC for the 99%
High-performance computing for the long tail of science

- Comet goals (from NSF 13-528 solicitation)
  - “… expand the use of high end resources to a much larger and more diverse community
  - … support the entire spectrum of NSF communities
  - ... promote a more comprehensive and balanced portfolio
  - … include research communities that are not users of traditional HPC systems.“
HPC for the 99%

- 99% of jobs run on NSF’s HPC resources in 2012 used <2,048 cores
- And consumed >50% of the total core-hours across NSF resources
Key Strategies for Comet Users

• Target modest-scale users and new users/communities: goal of 10,000 users/year!

• Support capacity computing, with a system optimized for small/modest-scale jobs and quicker resource response using allocation/scheduling policies

• Build upon and expand efforts with Science Gateways, encouraging gateway usage and hosting via software and operating policies

• Provide a virtualized environment to support development of customized software stacks, virtual environments, and project control of workspaces
Comet: System Characteristics

- Total peak flops 2 PF
- Dell primary integrator
  - Intel Haswell processors w/ AVX2
  - Mellanox FDR InfiniBand
- 1,944 standard compute nodes (47K cores)
  - Dual CPUs, each 12-core, 2.5 GHz
  - 128 GB DDR4 2133 MHz DRAM
  - 2*160GB GB SSDs (local disk)
- 36 GPU nodes (Feb 2015)
  - Same as standard nodes plus
  - Two NVIDIA K80 cards, each with dual Kepler3 GPUs
- 4 large-memory nodes (April 2015)
  - 1.5 TB DDR4 1866 MHz DRAM
  - Four Haswell processors/node
- Hybrid fat-tree topology
  - FDR (56 Gbps) InfiniBand
  - Rack-level (72 nodes, 1,728 cores) full bisection bandwidth
  - 4:1 oversubscription cross-rack
- Performance Storage (Aeon)
  - 7.6 PB, 200 GB/s; Lustre
  - Scratch & Persistent Storage segments
- Durable Storage (Aeon)
  - 6 PB, 100 GB/s; Lustre
  - Automatic backups of critical data
- Gateway hosting nodes
- Virtual image repository
- Home directory storage
- 100 Gbps external connectivity to Internet2 & ESNet
Comet Network Architecture

InfiniBand compute, Ethernet Storage

**Node-Local Storage**
- 320 GB
- 72 HSWL
- 36 GPU
- 4 Large-Memory

**Performance Storage**
- 7 PB, 200 GB/s
- 32 storage servers

**Durable Storage**
- 6 PB, 100 GB/s
- 64 storage servers

- 7x 36-port FDR in each rack wired as full fat-tree. 4:1 over subscription between racks.

**Core InfiniBand**
- (2 x 108-port)

**Mid-tier InfiniBand**
- 18 switches

**IB-Ethernet Bridges**
- (4 x 18-port each)

**Arista 40GbE**
- (2x)

**Data Movers**
- 27 racks
- FDR 36p
- 64 40GbE
- 128 10GbE

**Internet 2**
- Juniper 100 Gbps
- Arista 40GbE (2x)
- Data Mover Nodes

**Research and Education Network Access**
Data Movers

**Additional Support Components**
- (not shown for clarity)
- Ethernet Mgt Network (10 GbE)
- NFS Servers for Home Directories
- Virtual Image Repository
- Gateway/Portal Hosting Nodes
- Login Nodes
- Rocks Management Nodes

**SAN DIEGO SUPERCOMPUTER CENTER**
at the UNIVERSITY OF CALIFORNIA; SAN DIEGO
**Suggested Comet Applications**

- **Modest core counts**: full bisection bandwidth up to Comet island (1,728 cores)
- **128 GB DRAM/node (5.3 GB/core)**: single node shared memory apps and MPI codes with large per-process memory footprint
- **AVX2**: Codes with vectorizable loops. Any application with significant performance gain relative to Sandy Bridge or Ivy Bridge (AVX)
- **SSDs**: Computational chemistry, finite elements. Apps that generate large numbers of small temporary files (finance, QM/MM)
**Suggested Comet Applications, cont’d**

- **GPU nodes:** Molecular dynamics, linear algebra, image and signal processing.
  - Doesn’t replace Keeneland, but for workloads that have some GPU requirements.
- **Large memory nodes:** *de novo* genome assembly, visualization of large data sets, other large memory apps
- **Science Gateways:** Gateway-friendly environment with local gateway hosting capability, flexible allocations, scheduling policies for rapid throughput, heterogeneous workflows, and virtual clusters for software environment
- **High performance virtualization:** workloads with customized software stacks, especially those that are difficult to port or deploy in standard XSEDE environment
**Single Root I/O Virtualization in HPC**

- **Problem**: Virtualization generally has resulted in significant I/O performance degradation (e.g., excessive DMA interrupts)
- **Solution**: SR-IOV and Mellanox ConnectX-3 InfiniBand host channel adapters
  - One physical function → multiple virtual functions, each light weight but with its own DMA streams, memory space, interrupts
  - Allows DMA to bypass hypervisor to VMs
- **SRIOV enables virtual HPC cluster w/ near-native InfiniBand latency/bandwidth and minimal overhead**
Latency Results:
QDR IB & 10 GbE, native and SR-IOV

• SR-IOV with QDR InfiniBand
  • < 30% overhead for small messages (<128 bytes)
    • < 10% overhead for eager send/receive
  • Overhead → 0% for bandwidth-limited regime
• Amazon EC2 (10 GbE)
  • > 50X worse latency
  • Time dependent (noisy)

50x less latency than Amazon EC2

Figure 5. MPI point-to-point latency measured by osu_latency for QDR InfiniBand. Included for scale are the analogous 10GbE measurements from Amazon (AWS) and non-virtualized 10GbE.
**Bandwidth Results:**

**QDR IB & 10 GbE, native and SR-IOV**

- Comparison of bandwidth relative to native InfiniBand
- SR-IOV w/ QDR InfiniBand
  - < 2% bandwidth loss over entire range
  - > 95% peak bandwidth
- Amazon EC2 (10 GbE)
  - < 35% peak bandwidth
  - While ratio of QDR/10GbE bandwidth is ~4X, EC2 bandwidth is 9-25X worse than SR-IOV IB

10x more bandwidth than Amazon EC2

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**Figure 6.** MPI point-to-point bandwidth measured by osu_bw for QDR InfiniBand. Included for scale are the analogous 10GbE measurements from Amazon (AWS) and non-virtualized 10GbE.
WRF Weather Modeling – 15% Overhead with SR-IOV IB

- 96-core (6-node) calculation
- Nearest-neighbor communication
- Scalable algorithms
- SR-IOV incurs modest (15%) performance hit
- ... but still 20% faster than EC2
  - Despite 20% slower CPUs
Quantum ESPRESSO: 28% Overhead

- 48-core (3 node) calculation
- CG matrix inversion - irregular communication
- 3D FFT matrix transposes (all-to-all communication)
- 28% slower w/ SR-IOV vs native IB
- SR-IOV still > 500% faster than EC2
  - Despite 20% slower CPUs
High Level Schedule

- Dec 2014-Jan 2015
  - Build and component test
- Feb 2015
  - Friendly users
  - Integrated acceptance tests
  - NSF review panel
- March 2015
  - production