HPC ADVISORY COUNCIL

NAMD
Performance Benchmark and Profiling

February 2011

AMD The future is fusion

DELL

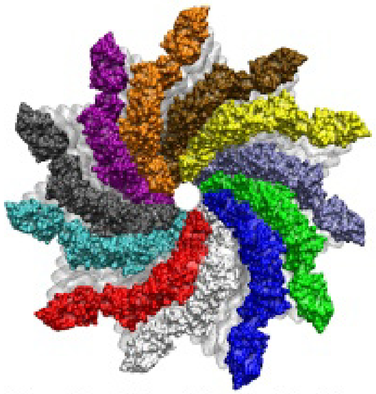
Mellanox TECHNOLOGIES

Note

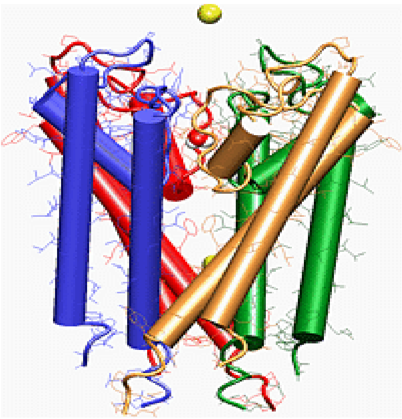
- **The following research was performed under the HPC Advisory Council activities**
  - Participating vendors: AMD, Dell, Mellanox
  - Compute resource - HPC Advisory Council Cluster Center
- **For more info please refer to**
  - http:// www.amd.com
  - http:// www.dell.com/hpc
  - http://www.mellanox.com
  - http://www.ks.uiuc.edu/Research/namd

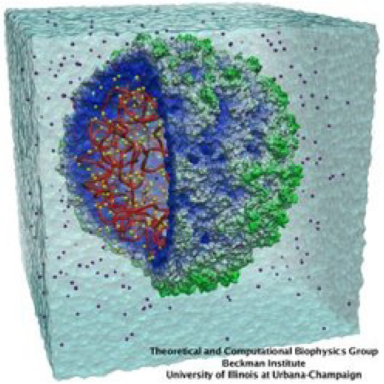
NAMD

- A parallel molecular dynamics code that received the 2002 Gordon Bell Award
- Designed for high-performance simulation of large biomolecular systems
  - **Scales to hundreds of processors and millions of atoms**
- Developed by the joint collaboration of the Theoretical and Computational Biophysics Group (TCB) and the Parallel Programming Laboratory (PPL) at the University of Illinois at Urbana-Champaign
- NAMD is distributed free of charge with source code



Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign





Theoretical and Computational Biophysics Group
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Objectives

- **The following was done to provide best practices**
  - NAMD performance benchmarking
  - Interconnect performance comparisons
  - Understanding NAMD communication patterns
  - Ways to increase NAMD productivity
  - Compilers and MPI libraries comparisons

- **The presented results will demonstrate**
  - The scalability of the compute environment
  - The capability of NAMD to achieve scalable productivity
  - Considerations for performance optimizations

Test Cluster Configuration

- Dell™ PowerEdge™ R815 11-node (528-core) cluster
- AMD™ Opteron™ 6174 (code name “Magny-Cours”) 12-cores @ 2.2 GHz CPUs
- 4 CPU sockets per server node
- Mellanox ConnectX-2 VPI adapters for 40Gb/s QDR InfiniBand and 10Gb/s Ethernet
- Mellanox MTS3600Q 36-Port 40Gb/s QDR InfiniBand switch
- Fulcrum based 10Gb/s Ethernet switch
- Memory: 128GB memory per node DDR3 1333MHz
- OS: RHEL 5.5, MLNX-OFED 1.5.2 InfiniBand SW stack
- MPI: MVAPICH2-1.6RC2, Open MPI 1.4.3, Platform MPI 8.0.1
- Compilers: GNU Compilers 4.1.2
- Application: NAMD 2.7 (External libraries used: charm-6.2.2, fftw-2.1.3, TCL 8.3)
- Benchmark workload: ApoA1 bloodstream lipoprotein particle model (92,224 atoms, 12A cutoff)

Dell™ PowerEdge™ R815 11-node cluster

- **HPC Advisory Council Test-bed System**

- **New 11-node 528 core cluster - featuring Dell PowerEdge™ R815 servers**
  - Replacement system for Dell PowerEdge SC1435 (192 cores) cluster system following 2 years of rigorous benchmarking and product EOL
    - System to be redirected to explore HPC in the Cloud applications

- **Workload profiling and benchmarking**
  - Characterization for HPC and compute intense environments
  - Optimization for scale, sizing and configuration and workload performance
  - Test-bed Benchmarks
    - RFPs
    - Customers/Prospects, etc
  - ISV & Industry standard application characterization
  - Best practices & usage analysis

About Dell PowerEdge™ Platform Advantages

Best of breed technologies and partners

Combination of AMD™ Opteron™ 6100 series platform and Mellanox ConnectX InfiniBand on Dell HPC

Solutions provide the ultimate platform for speed and scale

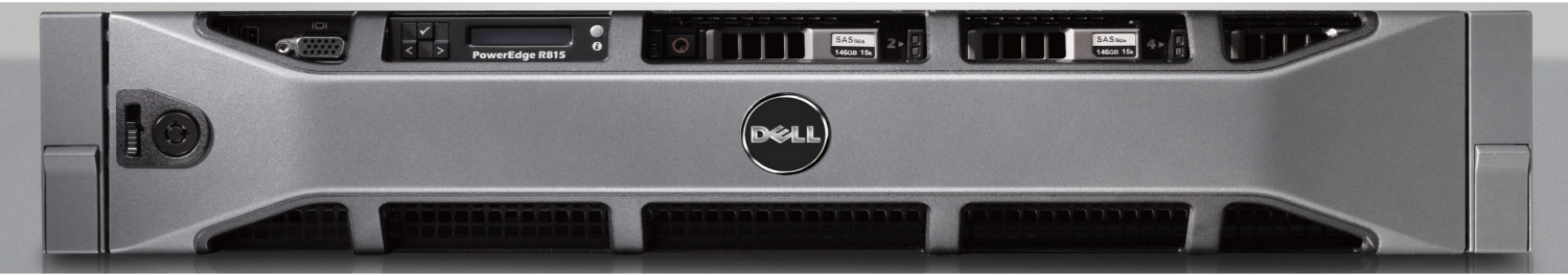
- Dell PowerEdge R815 system delivers 4 socket performance in dense 2U form factor
- Up to 48 core/32DIMMs per server – 1008 core in 42U enclosure

Integrated stacks designed to deliver the best price/performance/watt

- 2x more memory and processing power in half of the space
- Energy optimized low flow fans, improved power supplies and dual SD modules

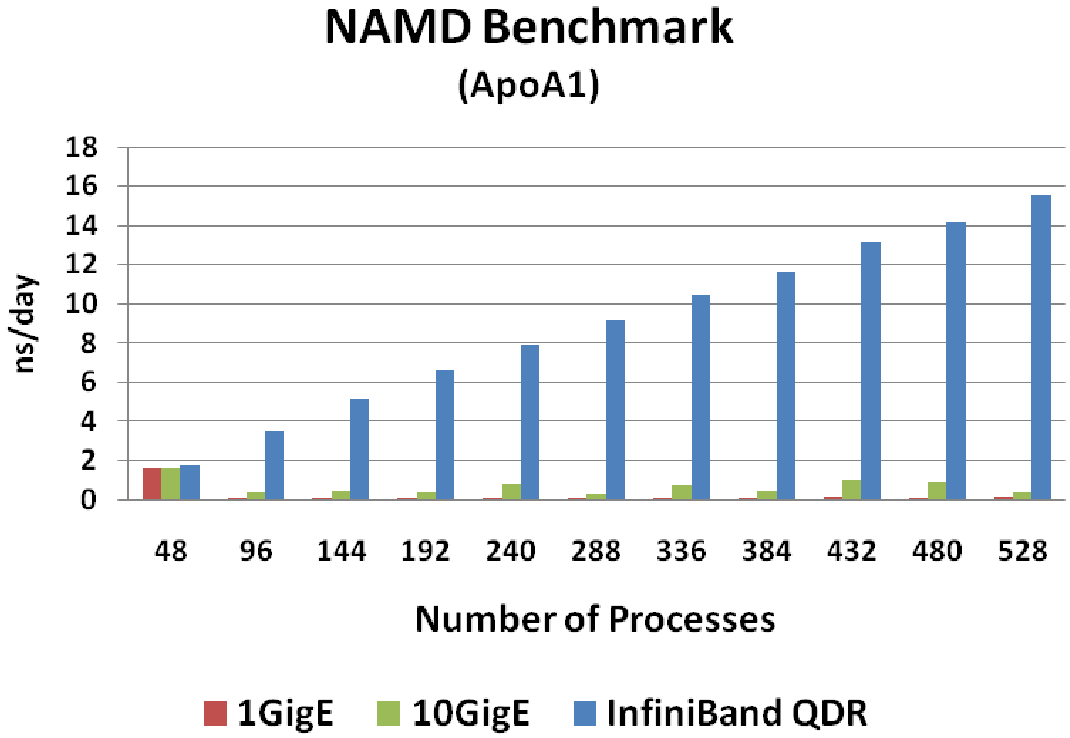
Optimized for long-term capital and operating investment protection

- System expansion
- Component upgrades and feature releases



NAMD Performance – Interconnects

- **InfiniBand shows continuous gain as the cluster scales**
- **Ethernet performance does not scale beyond 48 cores**

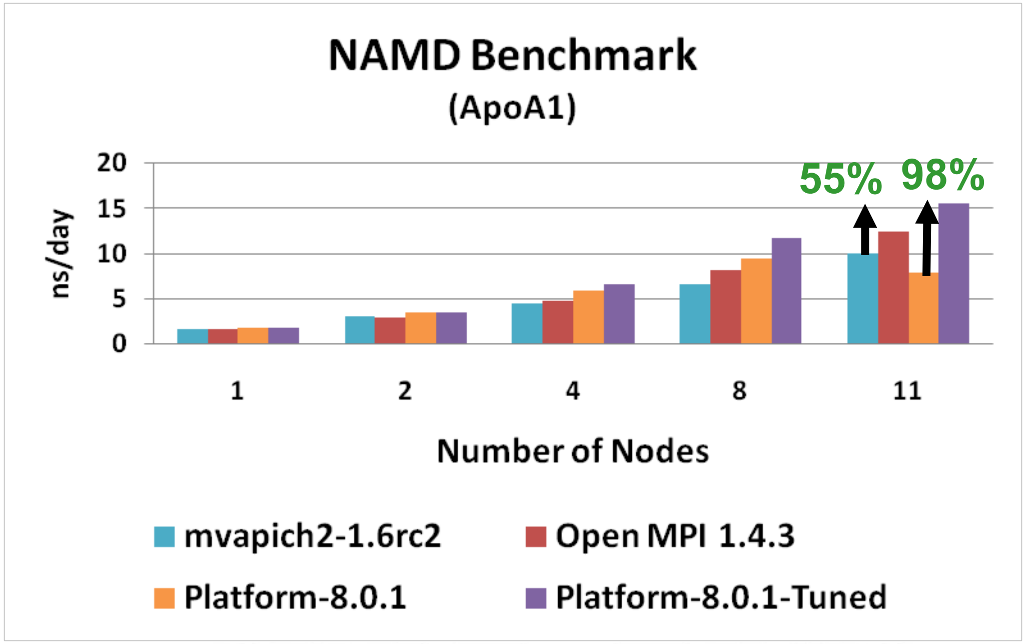


Higher is better

48 Cores/Node

NAMD Performance – MPI Implementations

- **Tuned Platform MPI performs the best**
  - Up to 55% faster than MVAPICH2 at 528 processes
  - Up to 98% improvement over the un-tuned version
    - Un-tuned version hit by performance limitation after 512-core
  - Tuned RDMA message sizes, Shared Receive Queue and related env-vars:
    - -srq -IBV -aff=automatic -e MPI_RDMA_MSGSIZE=16384,16384,4194304 -e MPI_RDMA_NSRQRECV=2048 -e MPI_RDMA_NFRAGMENT=128

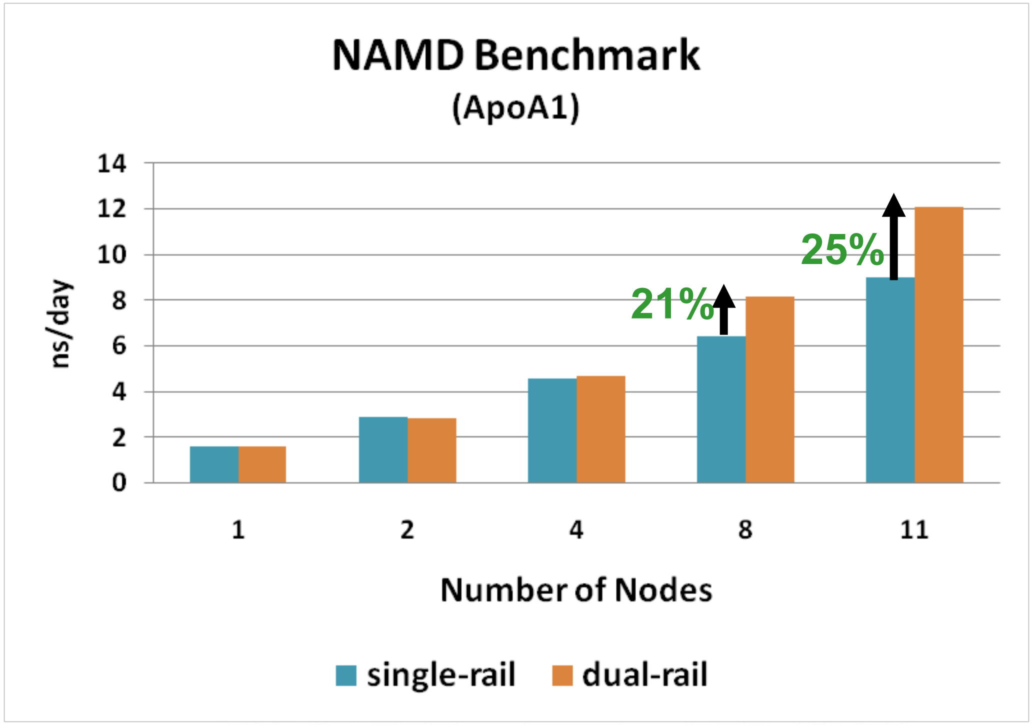


Higher is better

48 Cores/Node

NAMD Performance – InfiniBand Multi-rail

- **Dual-rail (Dual InfiniBand cards) enables better performance than single-rail**
  - Up to 25% better at 11-node
- **The benefit of dual-rail starts to emerge at 8-node**
  - As message profiling shows the volume of messages begins to increase
- **Dual-rail enables round-robin of small messages on the 2 InfiniBand ports**



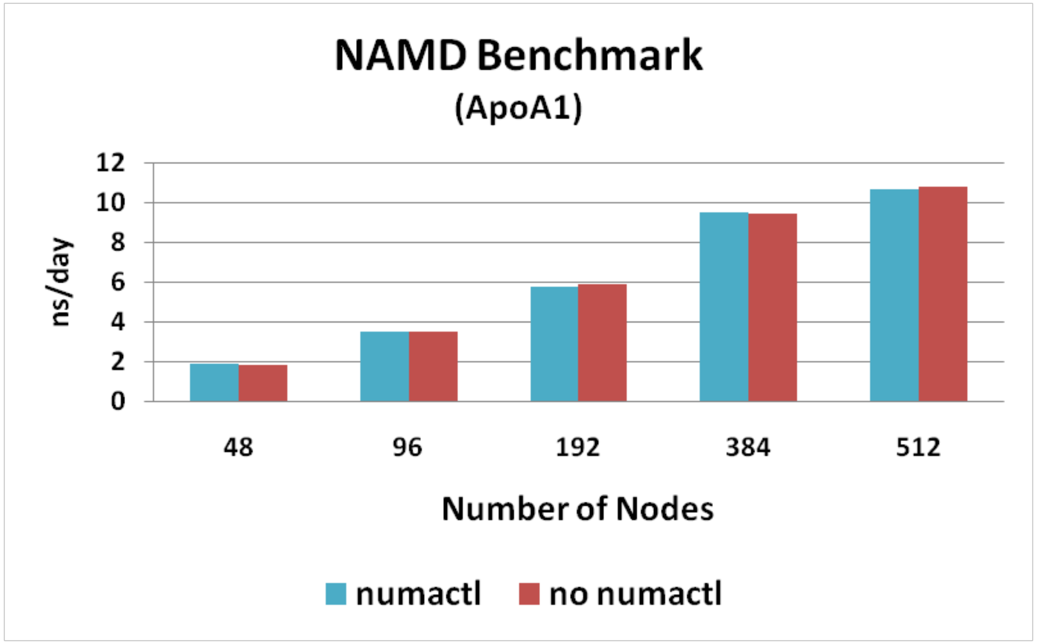
Higher is better

Open MPI

48 Cores/Node

NAMD Performance – Numactl

- **NUMA**
  - Stands for **Non-Uniform Memory Architecture**
  - Memory access depends on memory location relative to a processor
- **Numactl allows assigning processes to CPU node with local memory**
  - Results show no difference in job performance when assigning memory assignment

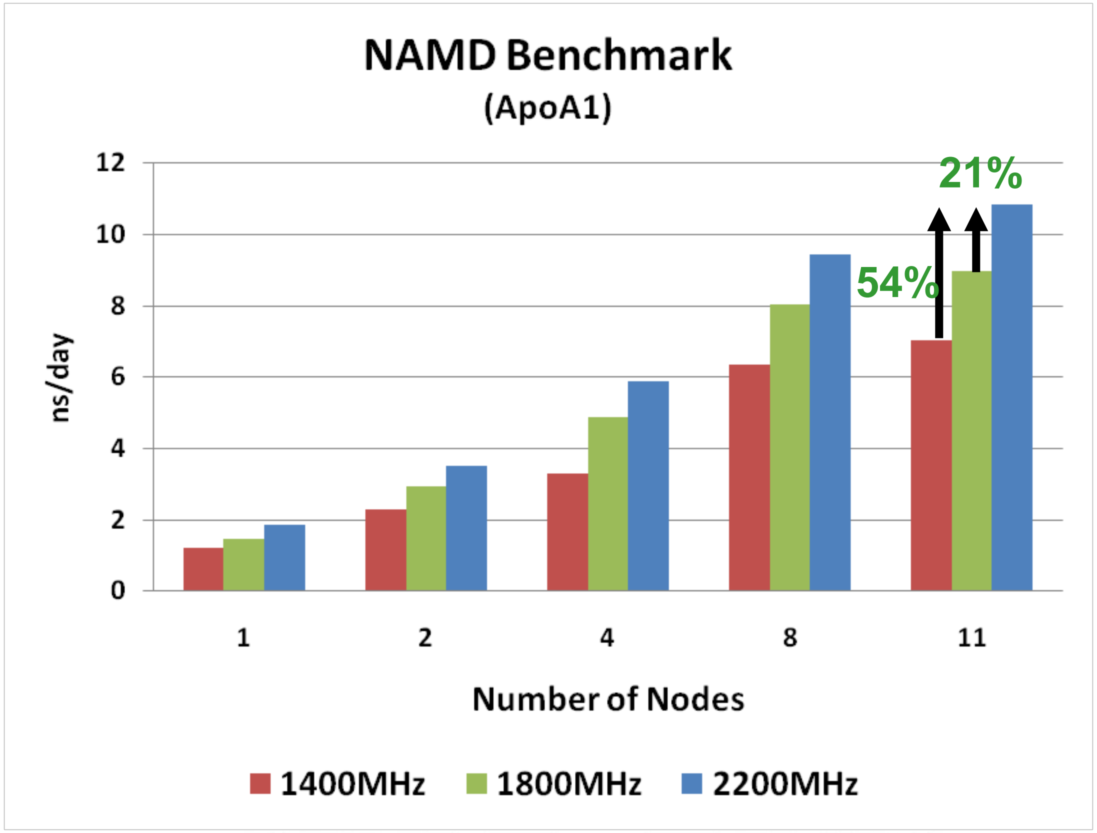


Higher is better

48 Cores/Node

NAMD Performance – CPU Frequency

- **Increasing CPU core frequency has a direct impact on job efficiency**
  - Up to 54% better job performance between 2200MHz vs 1400MHz
  - Up to 21% better job performance between 2200MHz vs 1800MHz
  - Performance improvement similar to the speed improvement

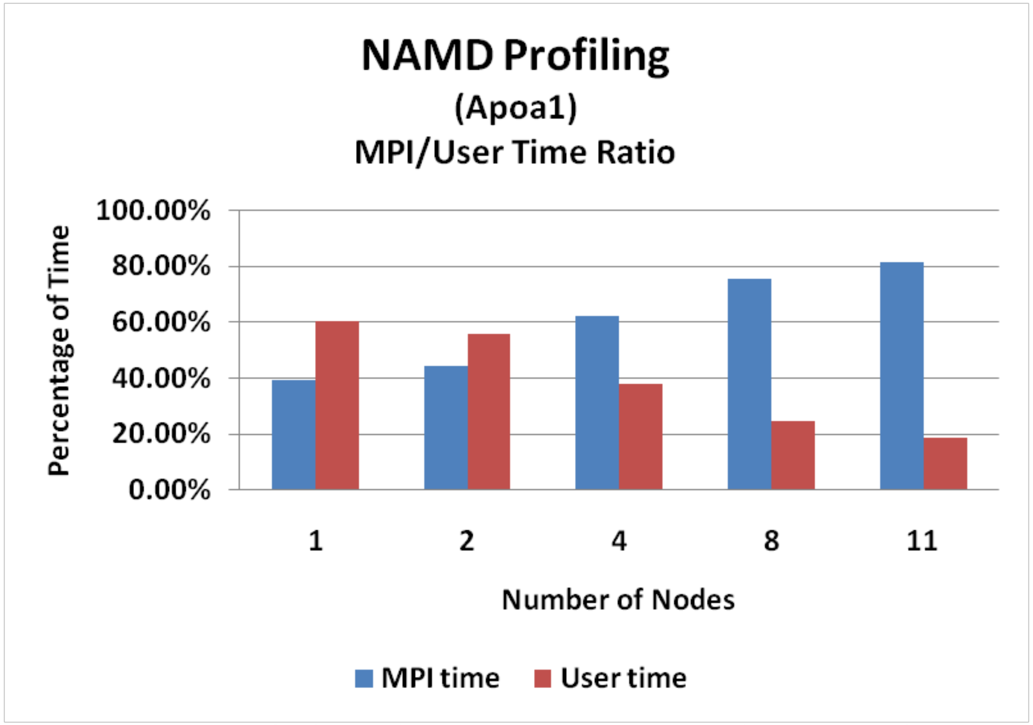


Higher is better

48 Cores/Node

NAMD Profiling – MPI/User Time Ratio

- **NAMD becomes highly communicative starting with 2-node**
  - Due to the high core counts per node
- **MPI communication time dominates the overall time**
  - Shows low latency interconnect such as InfiniBand is required for good scalability

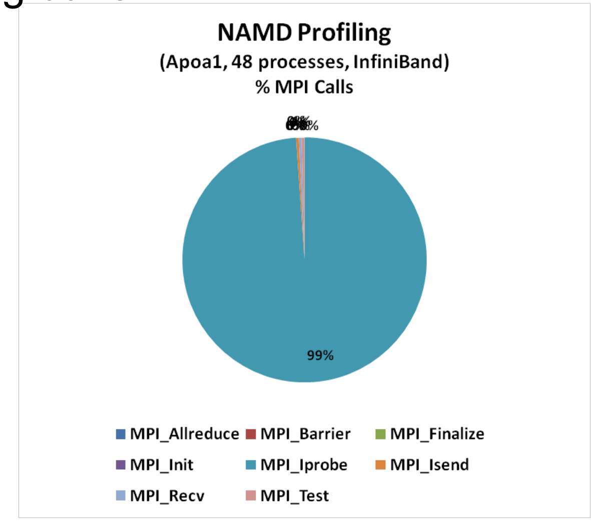


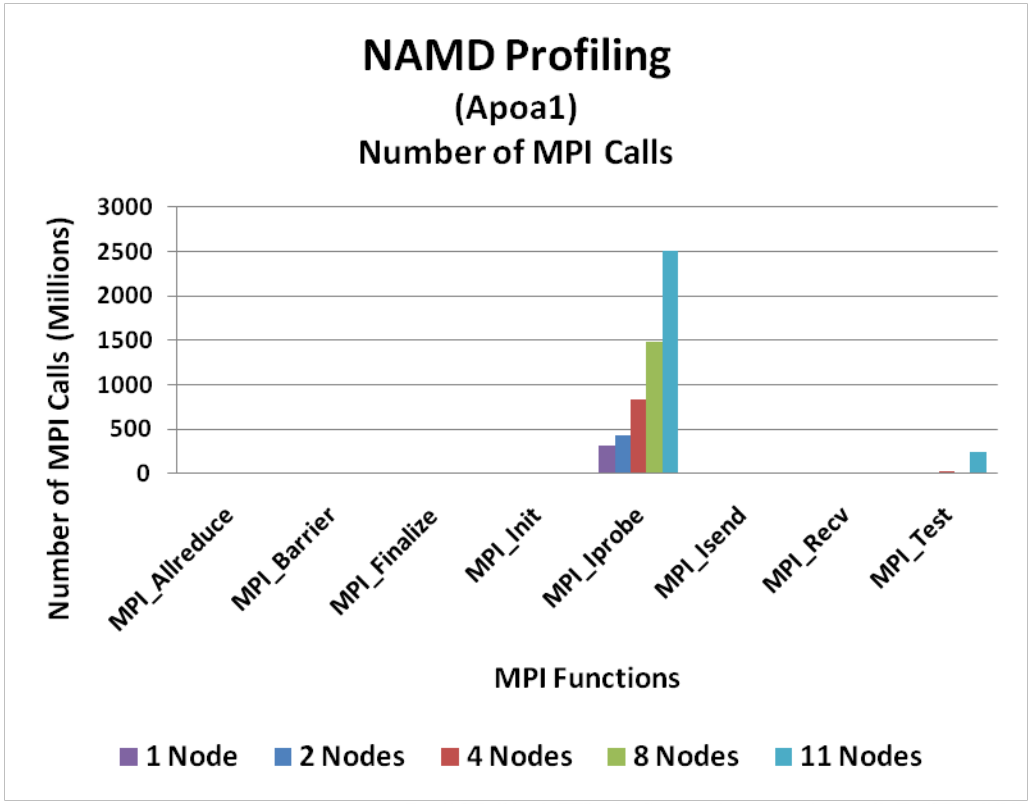
Higher is better

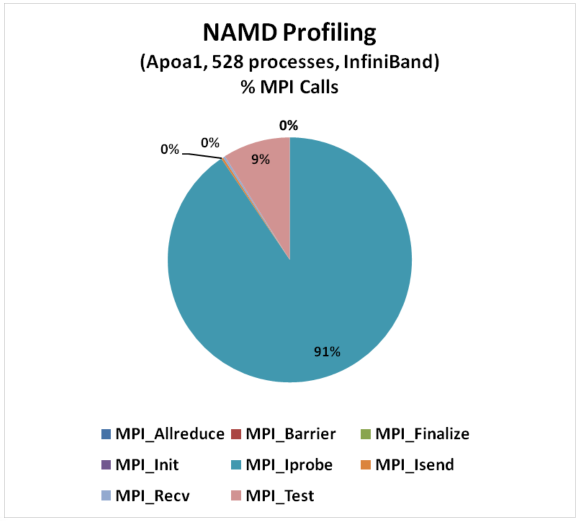
48 Cores/Node

NAMD Profiling – Number of MPI Calls

- **The most used MPI function is MPI_Iprobe**
  - Used for getting receiving message sizes and allows allocating buffer
  - Accounted for 99% of all MPI functions on a 1-node job
  - Accounted for 91% of all MPI functions on a 11-node job

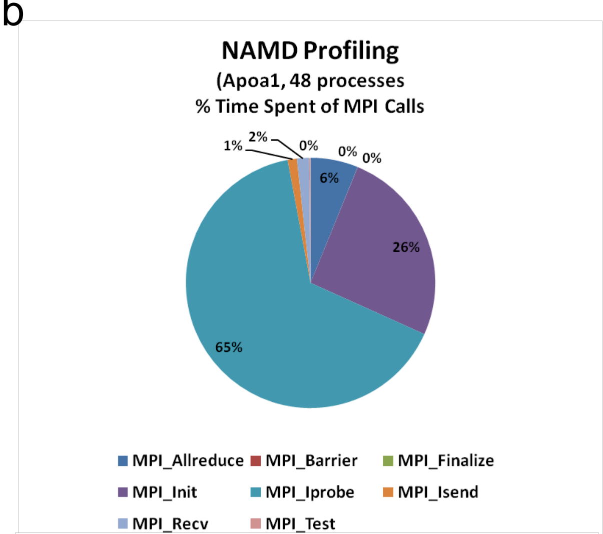


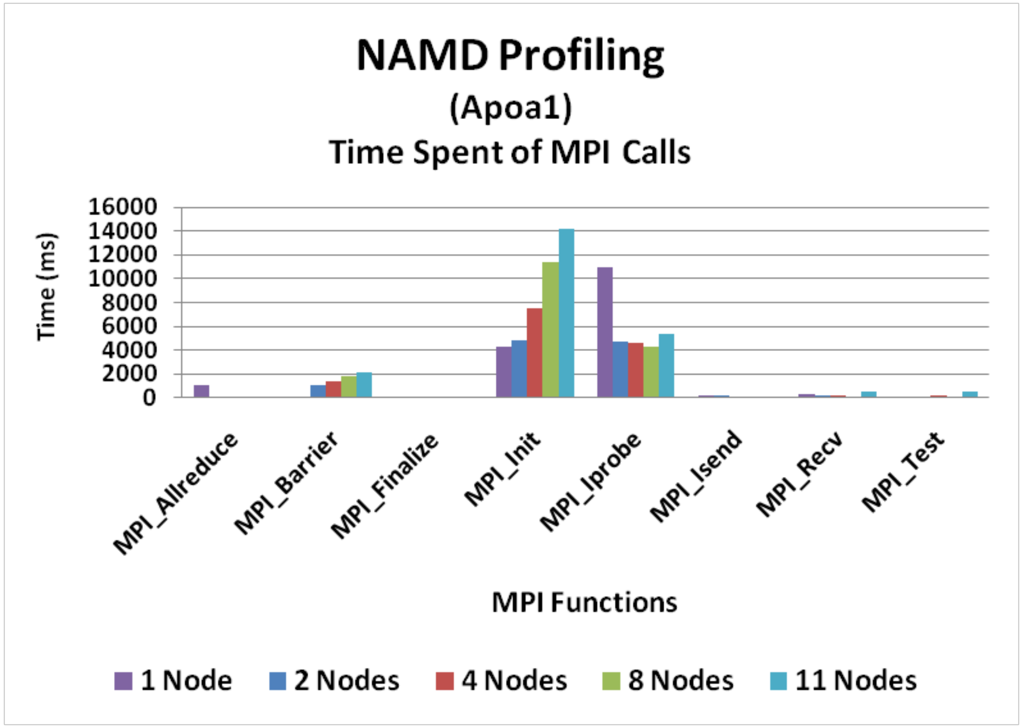


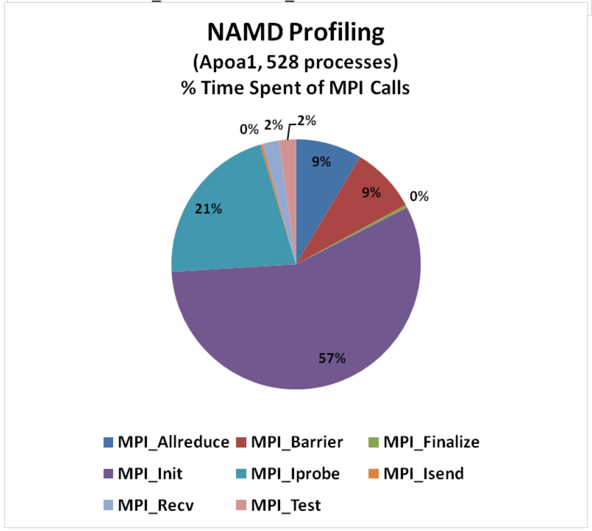


NAMD Profiling – Time Spent of MPI Calls

- **The most used MPI functions are MPI_Init and MPI_Iprobe**
  - Each accounted for 38% of all MPI functions on a 14-node job
- **MPI_Init occupies the largest percentage time**
  - Relatives to other MPI calls
  - Reflects other MPI data transfers are accomplished efficiently

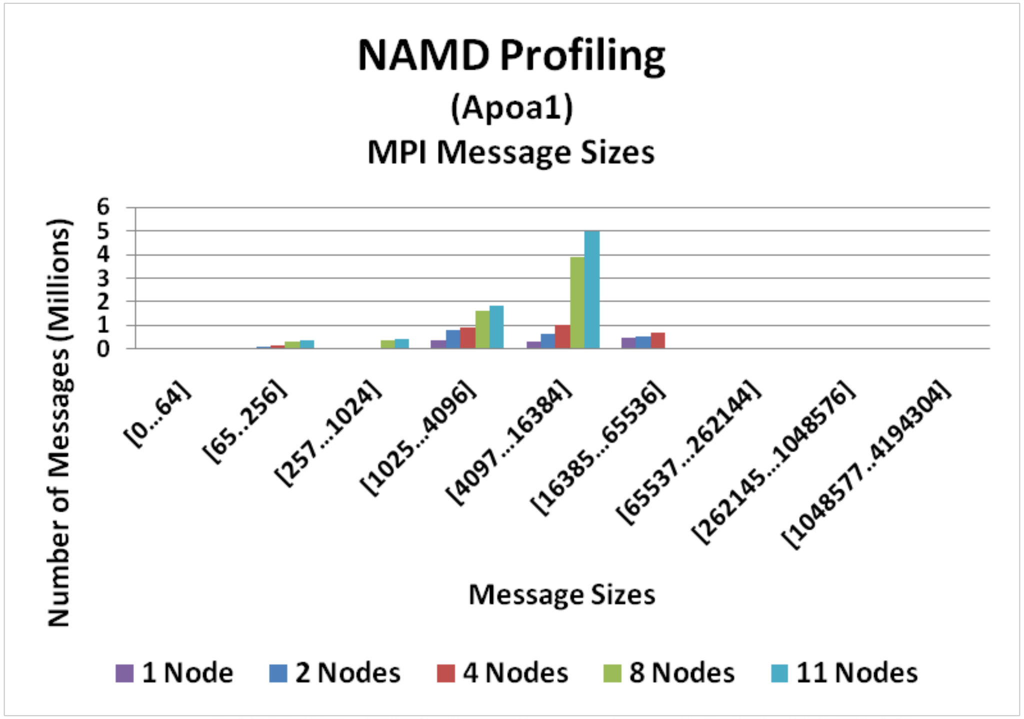






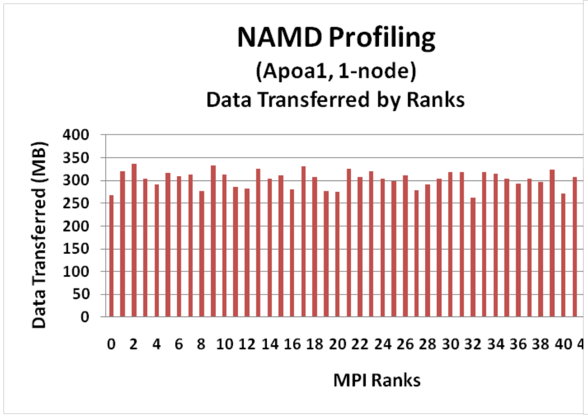
NAMD Profiling – MPI Message Sizes

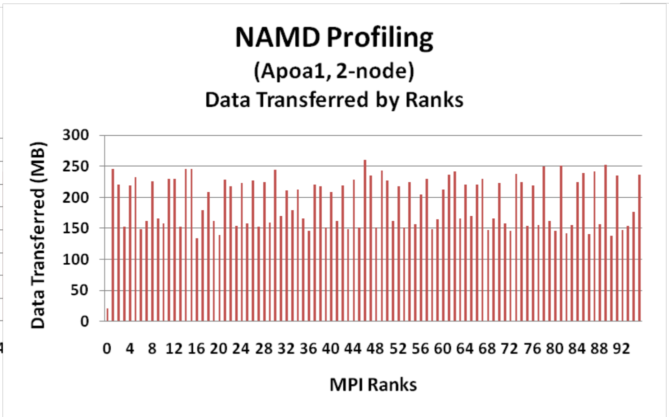
- **Majority of the MPI message sizes are**
  - in the range from 4KB to 16KB
- **Messages increase accelerates with the node count increases**
- **Benefit of Multi-rail begins to emerge starting with 8-node**

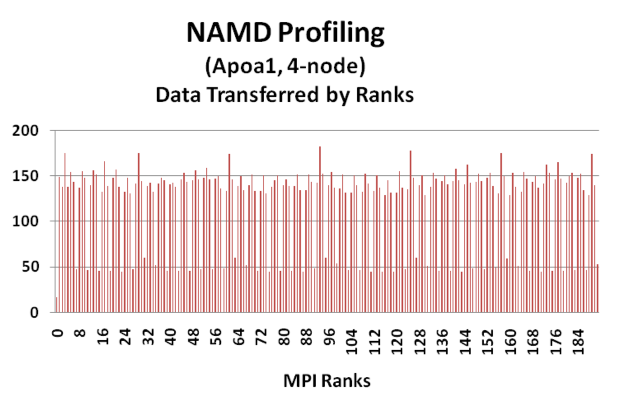


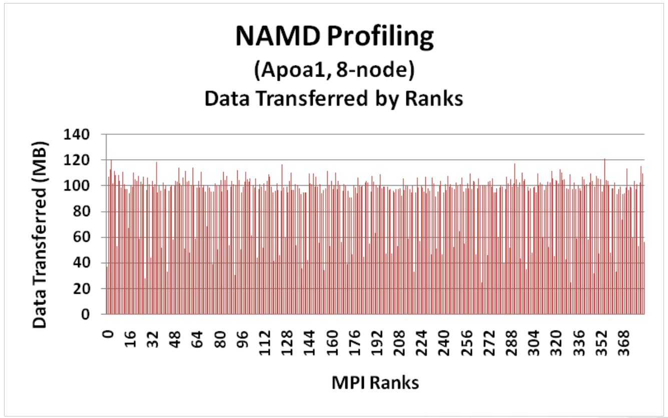
NAMD Profiling – Data Transfer Per Process

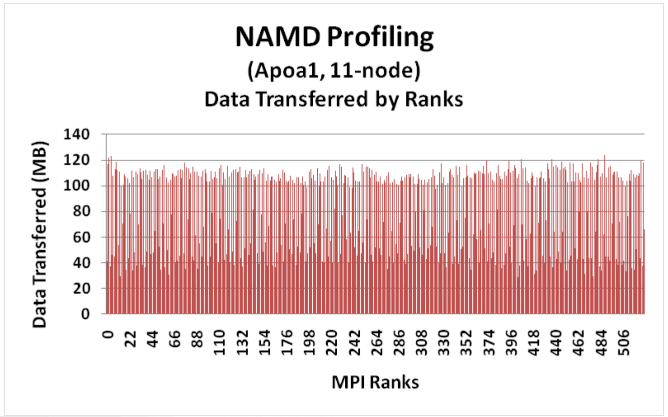
- **Data transferred to each MPI rank is showing some variance**
  - But overall data transfer is roughly the same on a per-node basis
- **As the cluster scales, less data is driven to each rank and each node**
  - 300MB per rank in a 48-process job versus 40-100MB per rank in a 528-process job





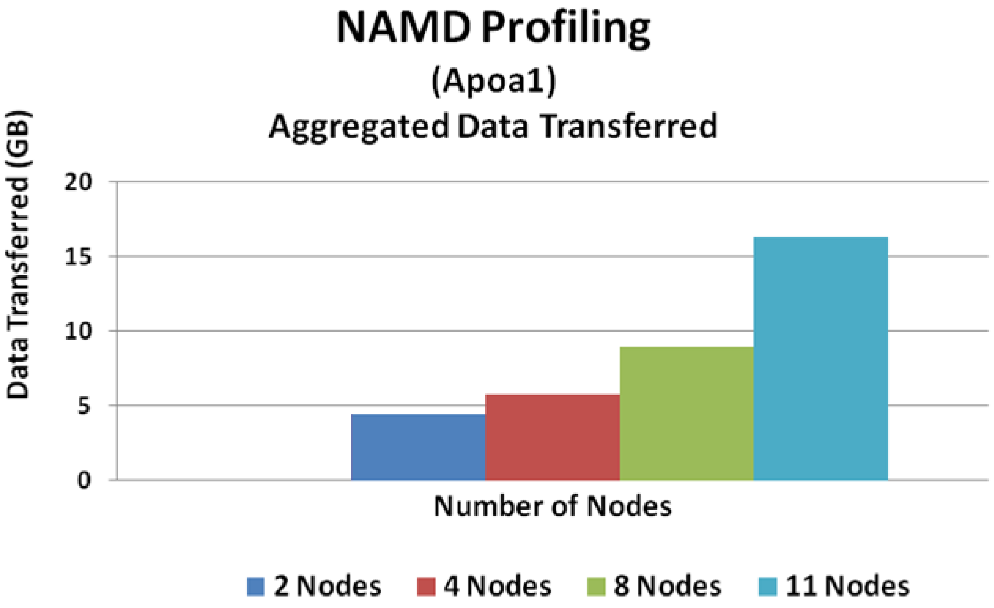






NAMD Profiling – Aggregated Data Transfer

- **Aggregated data transfer refers to:**
  - Total amount of data being transferred in the network between all MPI ranks collectively
- **The total data transfer increases as the cluster scales**
- **Demonstrates the advantage and importance of scalable network interconnect**
  - InfiniBand QDR can deliver bandwidth needed to push 16GB of data across the network



InfiniBand QDR

Summary

- **NAMD is an application for high-performance simulation of large biomolecular systems, is distributed free of charge with source code**
  - One of the leading bioscience application, found in many RFPs as well
- **Networking:**
  - InfiniBand shows as the preferred interconnect solution for any cluster size
    - Due to latency/throughput requirements,
  - Clear benefit for using dual-rail InfiniBand from 8-nodes and up
- **CPU:**
  - The CPU frequency has a direct impact on job productivity
- **MPIs:**
  - Open MPI (open source) and Platform MPI (commercial) are good candidates
  - Depends on the cluster size

Thank You

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