



NETWORK OF EXPERTISE

# NAMD Performance Benchmarks and Profiling

January 2009



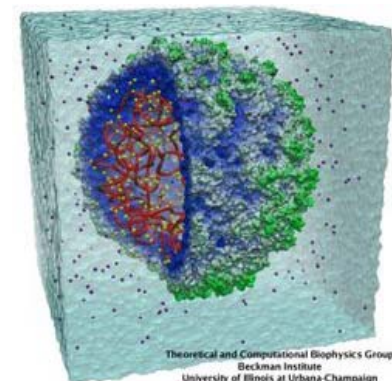
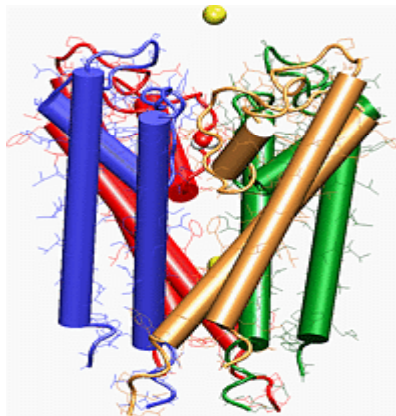
- **The following research was performed under the HPC Advisory Council activities**
  - AMD, Dell, Mellanox
  - HPC Advisory Council Cluster Center
- **For more info please refer to**
  - [www.mellanox.com](http://www.mellanox.com), [www.dell.com/hpc](http://www.dell.com/hpc), [www.amd.com](http://www.amd.com)

# NAMD

- A parallel, object-oriented molecular dynamics software
- Designed for high-performance simulation of large biomolecular systems
  - **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



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- **The presented research was done to provide**
  - NAMD performance benchmarking
  - Cluster Interconnect effect on NAMD performance
  - NAMD performance comparison with different MPI libraries
  - Understanding NAMD communication pattern
  - Productivity optimization

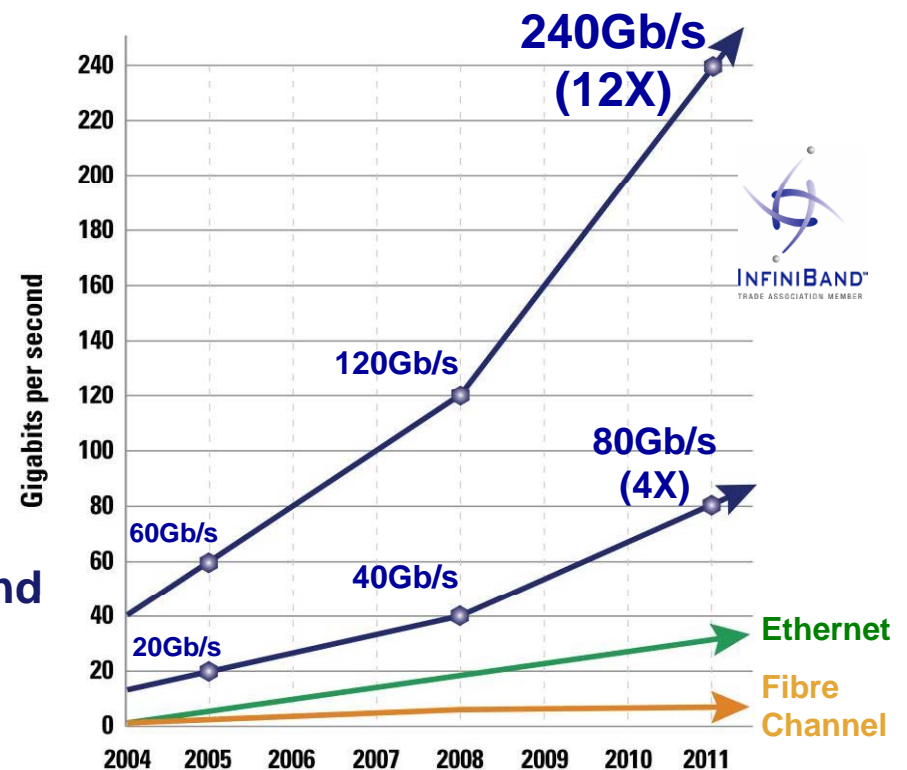
# Test Cluster Configuration

- **Dell™ PowerEdge™ SC 1435 24-node cluster**
- **Quad-Core AMD Opteron™ 2382 (code name Shanghai) CPUs**
- **Mellanox® InfiniBand ConnectX® DDR HCAs**
- **Mellanox® InfiniBand DDR Switch**
- **Memory: 16GB memory, DDR2 800MHz per node**
- **OS: RHEL5U2, OFED 1.4 InfiniBand SW stack**
- **MPI: Open MPI 1.3, Platform MPI 5.6.4**
- **Application: NAMD 2.6 with fftw3 libraries and Charm++ 6.0**
- **Benchmark Workload**
  - ApoA1 (92,224 atoms, 12A cutoff)

# Mellanox InfiniBand Solutions

- **Industry Standard**
  - Hardware, software, cabling, management
  - Design for clustering and storage interconnect
- **Performance**
  - 40Gb/s node-to-node
  - 120Gb/s switch-to-switch
  - 1us application latency
  - Most aggressive roadmap in the industry
- **Reliable with congestion management**
- **Efficient**
  - RDMA and Transport Offload
  - Kernel bypass
  - CPU focuses on application processing
- **Scalable for Petascale computing & beyond**
- **End-to-end quality of service**
- **Virtualization acceleration**
- **I/O consolidation Including storage**

## The InfiniBand Performance Gap is Increasing



InfiniBand Delivers the Lowest Latency

# Quad-Core AMD Opteron™ Processor

- **Performance**

- Quad-Core

- Enhanced CPU IPC
- 4x 512K L2 cache
- 6MB L3 Cache

- Direct Connect Architecture

- HyperTransport™ Technology
- Up to 24 GB/s peak per processor

- Floating Point

- 128-bit FPU per core
- 4 FLOPS/clock peak per core

- Integrated Memory Controller

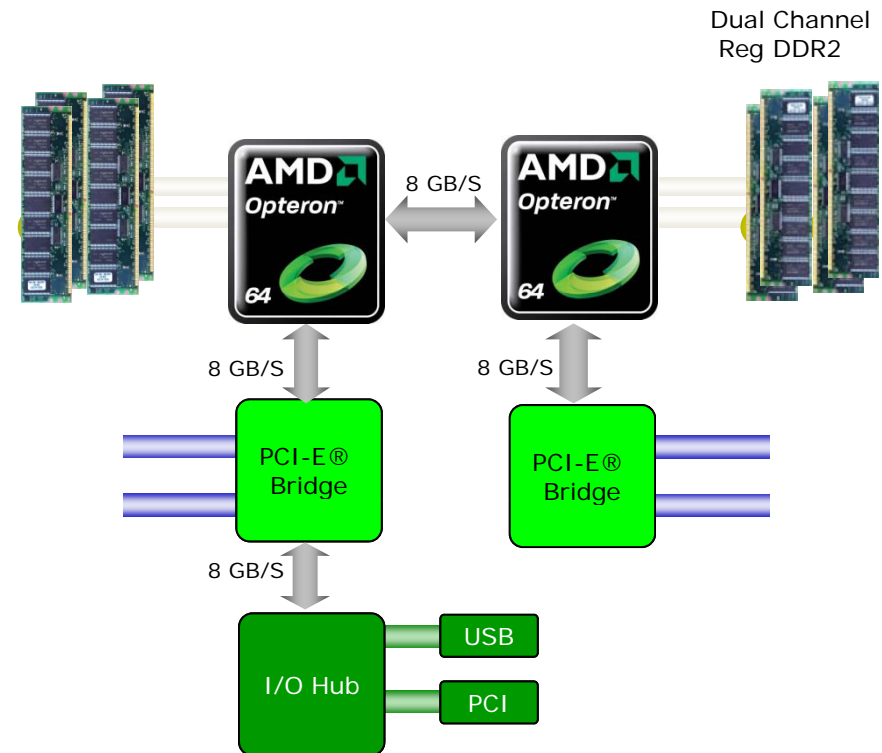
- Up to 12.8 GB/s
- DDR2-800 MHz or DDR2-667 MHz

- **Scalability**

- 48-bit Physical Addressing

- **Compatibility**

- Same power/thermal envelopes as 2<sup>nd</sup> / 3<sup>rd</sup> generation AMD Opteron™ processor



# Dell PowerEdge Servers helping Simplify IT

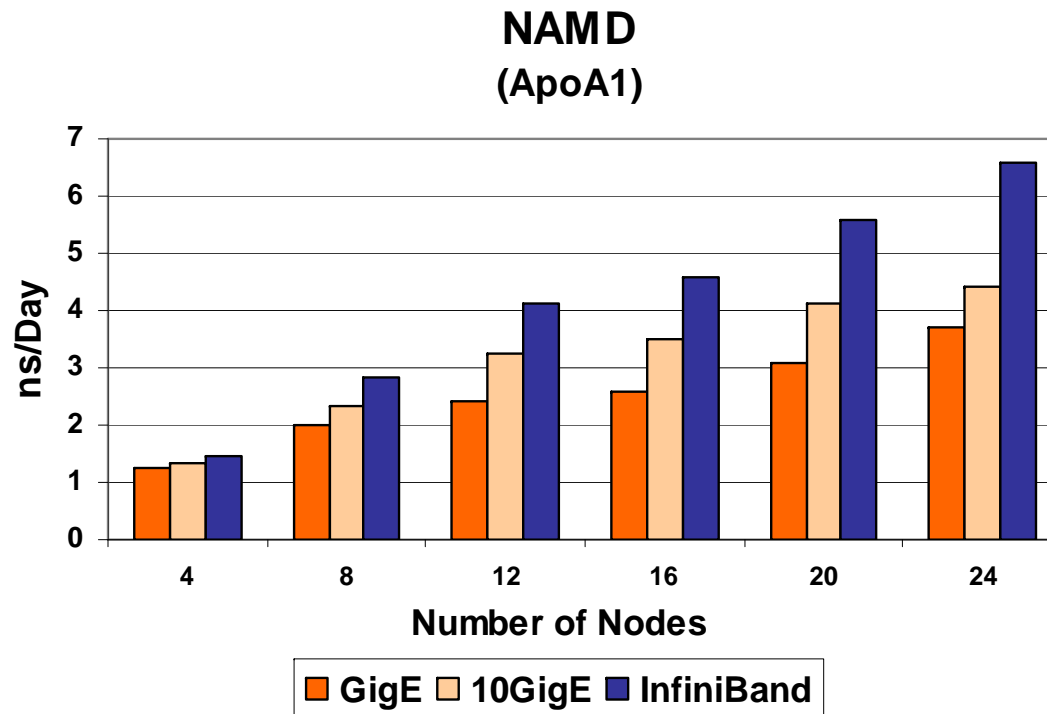
- **System Structure and Sizing Guidelines**
  - 24-node cluster build with Dell PowerEdge™ SC 1435 Servers
  - Servers optimized for High Performance Computing environments
  - Building Block Foundations for best price/performance and performance/watt
- **Dell HPC Solutions**
  - Scalable Architectures for High Performance and Productivity
  - Dell's comprehensive HPC services help manage the lifecycle requirements.
  - Integrated, Tested and Validated Architectures
- **Workload Modeling**
  - Optimized System Size, Configuration and Workloads
  - Test-bed Benchmarks
  - ISV Applications Characterization
  - Best Practices & Usage Analysis





# NAMD Results – ApoA1 Case

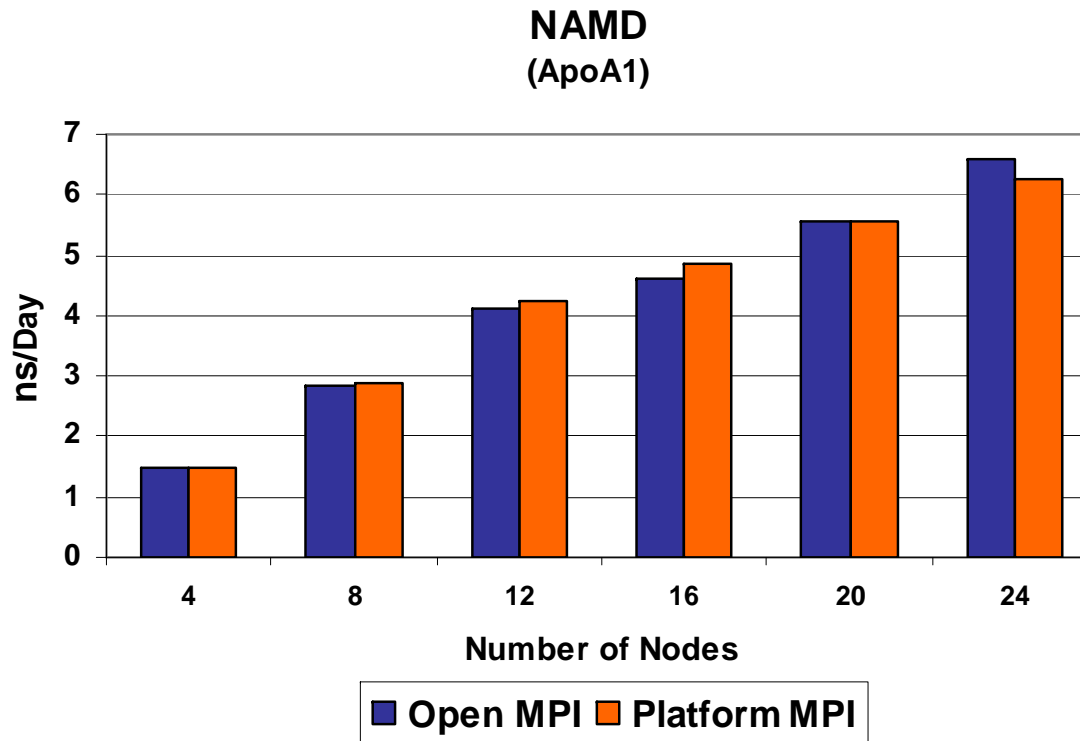
- **ApoA1 case - benchmark comprises 92K atoms of lipid, protein, and water**
  - Models a bloodstream lipoprotein particle
  - One of the most used data sets for benchmarking NAMD
- **InfiniBand 20Gb/s outperforms GigE and 10GigE in every cluster size**
  - InfiniBand provides higher performance up to 79% vs GigE and 49% vs 10GigE



Open MPI

# NAMD Performance Comparison - MPI

- **Platform MPI and Open MPI provides same level of performance**
  - Platform MPI has better performance for cluster size lower than 20 nodes
  - Open MPI becomes better with 24 nodes
    - Higher configurations than 24 nodes were not tested

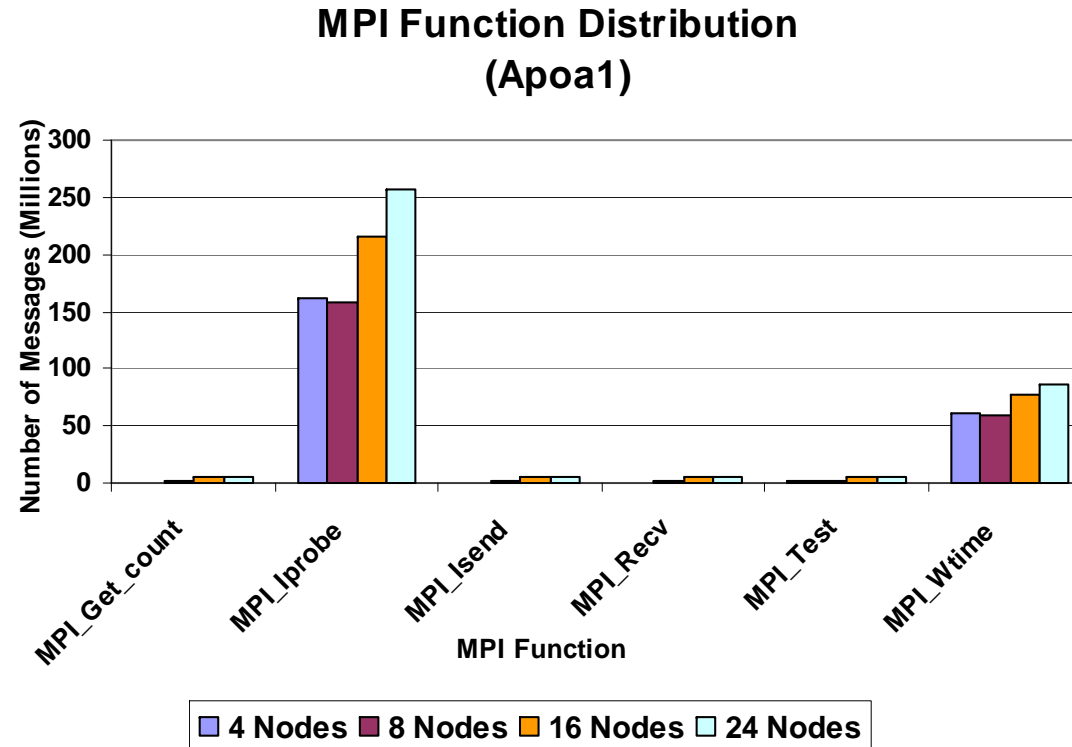


*Higher is better*

*These results are based on InfiniBand*

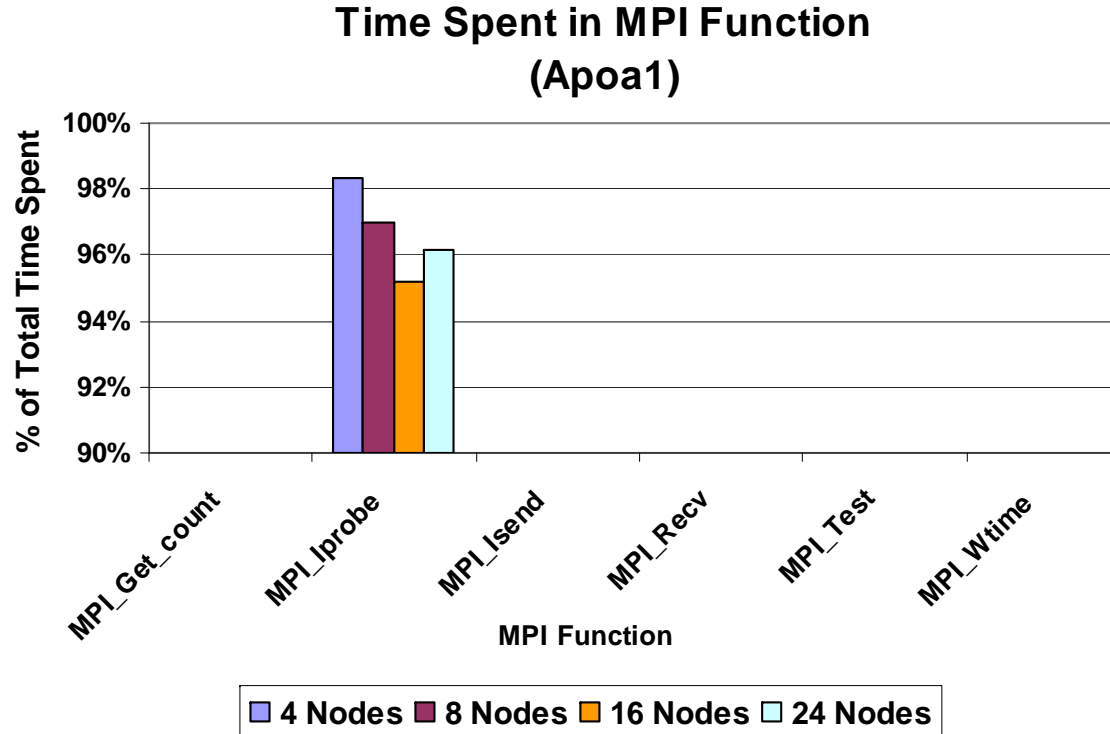
# MPI Functions in NAMD

- **MPI\_Iprobe is the most used MPI function in NAMD**
  - Number of MPI\_Iprobe messages increases dramatically with cluster size



# Time Spent in MPI Functions

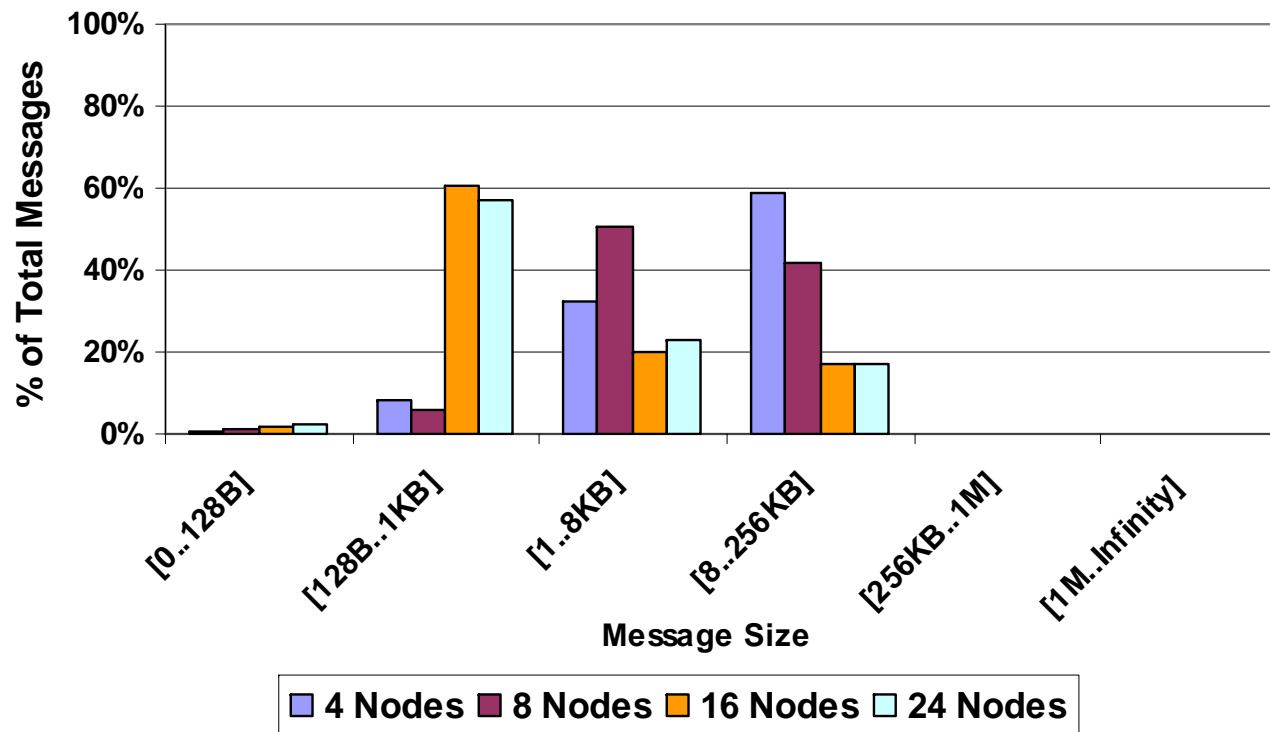
- **Majority of communication time is spent on MPI\_Iprobe**
  - Percentage are relative consistent as number of nodes increases



# Message Distribution

- As number of nodes scales, percentage of small messages increases
- Percentage of 1KB-256KB messages is relatively consistent for cluster sizes greater than 8 nodes
- Majority of the messages is in the range of 128B-1KB for cluster size greater than 8 nodes

**MPI Message Distribution  
(Apoa1)**

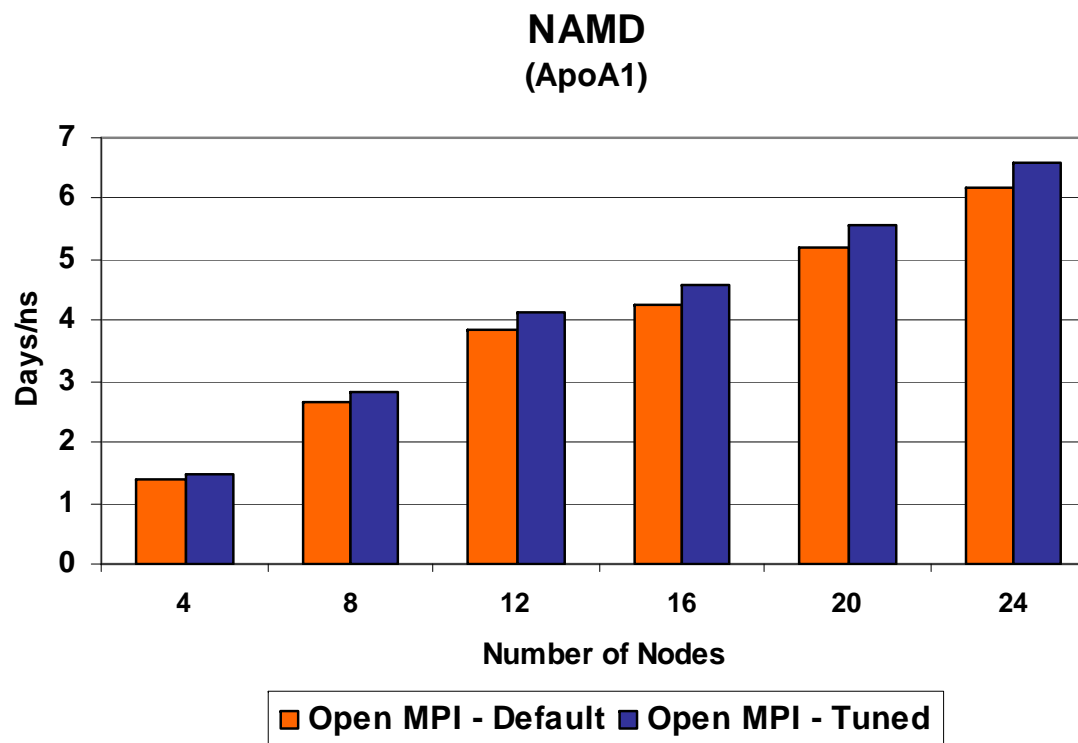


# NAMD Profiling Summary

- **NAMD was profiled to understand its communication pattern**
- **Message Size Distribution**
  - Most used message are ranging from 1KB to 8KB with node number less than 8
  - Percentage of mid size messages (128B to 1K) increases with cluster size
- **MPI function in NAMD**
  - MPI\_Iprobe is the key MPI function
  - MPI\_Iprobe counts up to 98% of total communication time
  - As cluster size scales, number of MPI\_Iprobe messages increases dramatically
- **Performance Optimization**
  - Tuning eager message passing parameters to minimize MPI\_Iprobe overhead

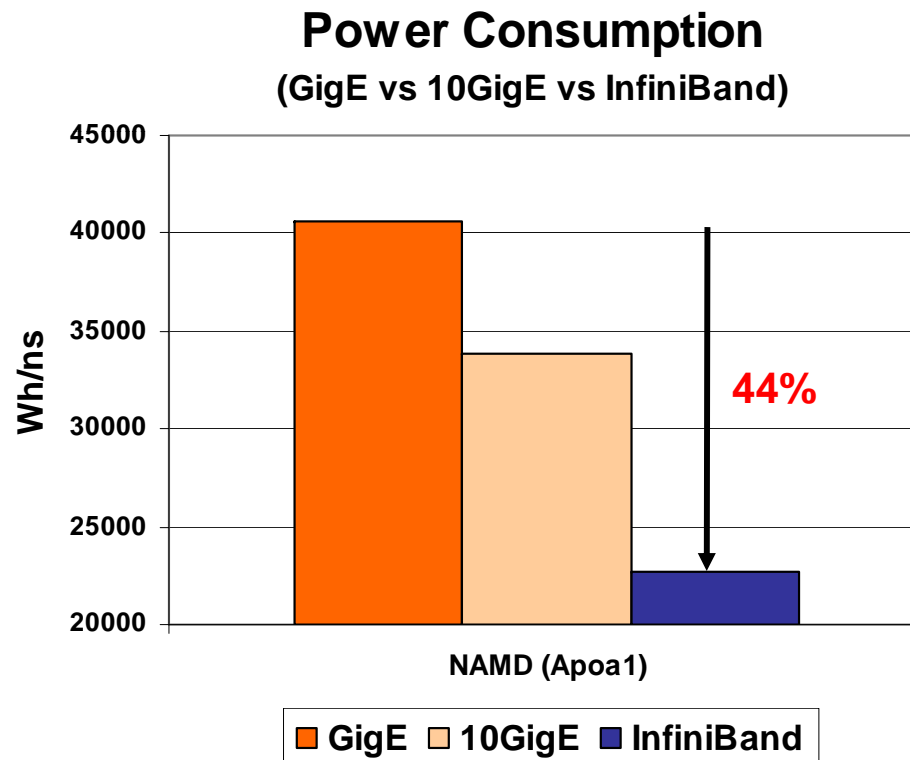
# Tuning MPI For Performance Improvements

- **MPI Performance tuning**
  - Enabling CPU affinity
    - `mca mpi_paffinity_alone 1`
  - Increasing eager limit over infiniband to 32K
    - `mca btl_openib_eager_limit 32767`
- **Performance increase of up to 10%**



# Power Consumption Comparison - Interconnect

- InfiniBand enables power efficient simulations
- Reducing system power consumption per job by up to 44%



24-node comparison

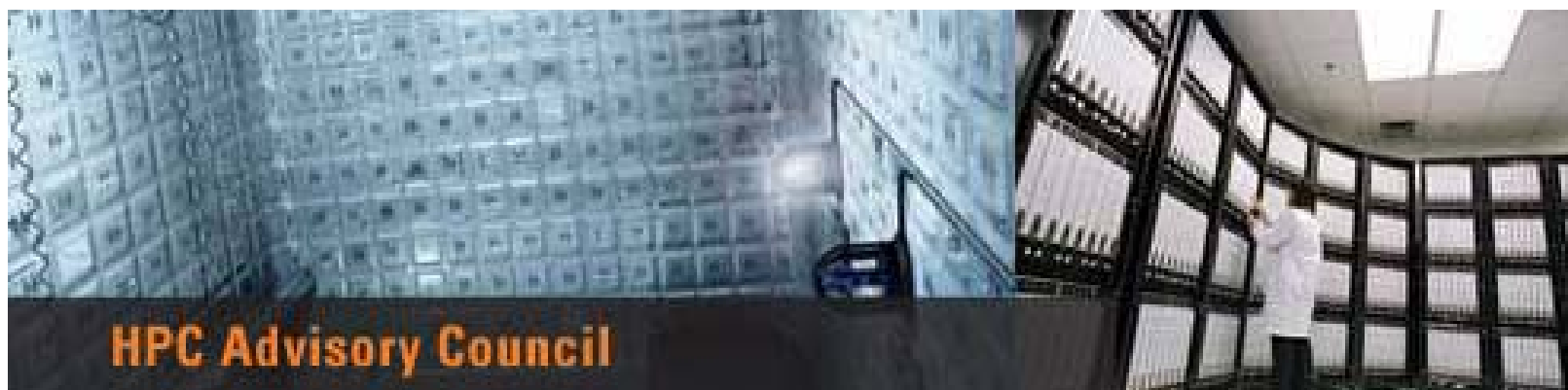


# Conclusions

- **NAMD relies on interconnect with low latency and high throughput**
  - Most messages transferred between processes are 128Bytes - 8KB messages
  - Number of messages scales up quickly as number of processes increases
- **InfiniBand enables NAMD performance scalability**
  - InfiniBand performance is up to 79% vs GigE and 49% vs 10GigE
- **NAMD attains similar performance with Platform MPI versus Open MPI**
  - MPI\_Iprobe performance affects NAMD performance
  - MPI tuning enables higher performance
- **Power Efficiency**
  - Less power consumed by finishing same amount of NAMD jobs
  - Saving in system power thus cooling

# Thank You

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