HPC ADVISORY COUNCIL

NAMD Performance Benchmark and Profiling

November 2010

hp

Mellanox TECHNOLOGIES

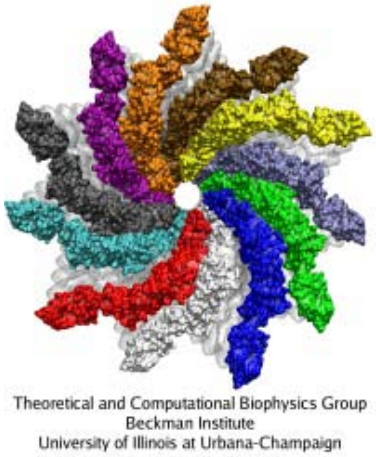
Note

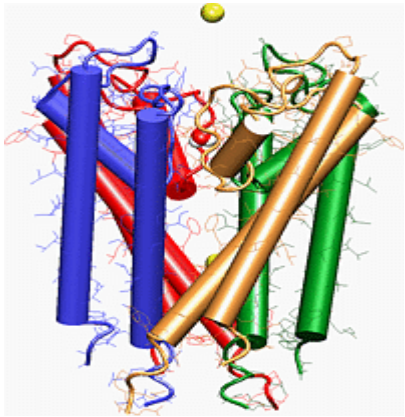
- **The following research was performed under the HPC Advisory Council activities**
  - Participating vendors: HP, Mellanox
  - Compute resource - HPC Advisory Council Cluster Center

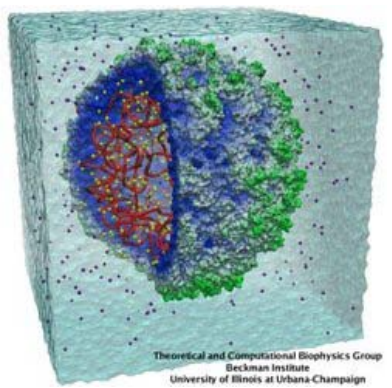
- **For more info please refer to**
  - www.mellanox.com
  - http://www.hp.com/go/hpc
  - http://www.ks.uiuc.edu/Research/namd

NAMD

- A parallel molecular dynamics code that received the 2002 Gordon Bell Award
- Designed for high-performance simulation of large biomolecular systems
- 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







Objectives

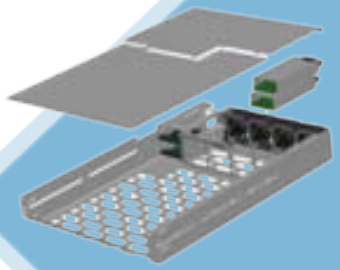
- **The presented research was done to provide best practices**
  - NAMD performance benchmarking
    - MPI libraries performance comparisons
    - Interconnect performance comparisons
  - Understanding NAMD communication patterns
  - Power-efficient simulations
- **The presented results will demonstrate**
  - The scalability of the compute environment
  - Considerations for power saving through balanced system configuration

Test Cluster Configuration

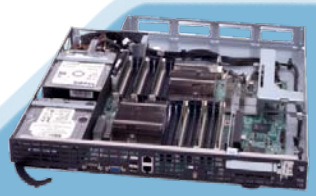
- **HP ProLiant SL2x170z G6 16-node cluster**
  - Six-Core Intel X5670 @ 2.93 GHz CPUs
  - Memory: 24GB per node
  - OS: CentOS5U4, OFED 1.5.1 InfiniBand SW stack
- **Mellanox ConnectX-2 adapters and switches**
- **Fulcrum based 10GigE switch**
- **MPI: Open MPI 1.4.1, MVAPICH-1.2.0**
- **Libraries: Charm++ 6.2.2**
- **Application: NAMD v2.7**
- **Benchmark Workload**
  - **STMV (Satellite tobacco mosaic virus) benchmark (1,066,628 atoms, periodic, PME)**

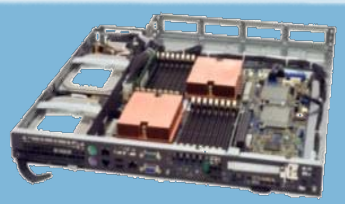
About HP ProLiant SL6000 Scalable System

- **Solution-optimized for extreme scale out**



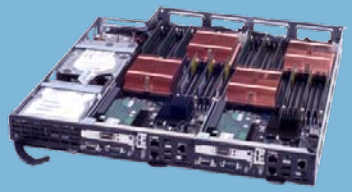
ProLiant z6000 chassis
Shared infrastructure
– fans, chassis, power





ProLiant SL160z G6 ProLiant SL165z G7
Large memory
-memory-cache apps

ProLiant SL170z G6
Large storage
-Web search and database apps



ProLiant SL2x170z G6
Highly dense
- HPC compute and
web front-end apps

Save on cost and energy -- per node, rack and data center

Mix and match configurations

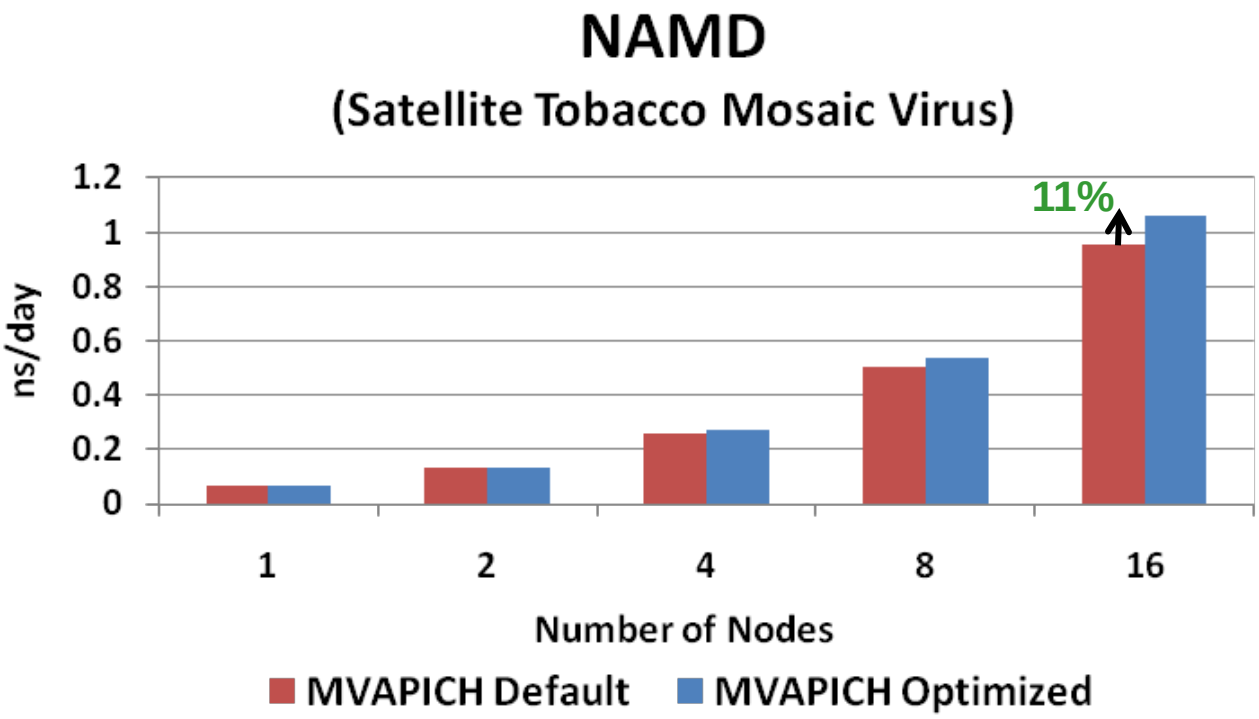
Deploy with confidence

#1 Power Efficiency*

* SPECpower_ssj2008
www.spec.org
17 June 2010, 13:28

NAMD Performance - MVAPICH

- **Performance improved by up to 11% with optimization**
  - VIADEV_RENDEZVOUS_THRESHOLD=50000
  - Advantage extends as node count increases

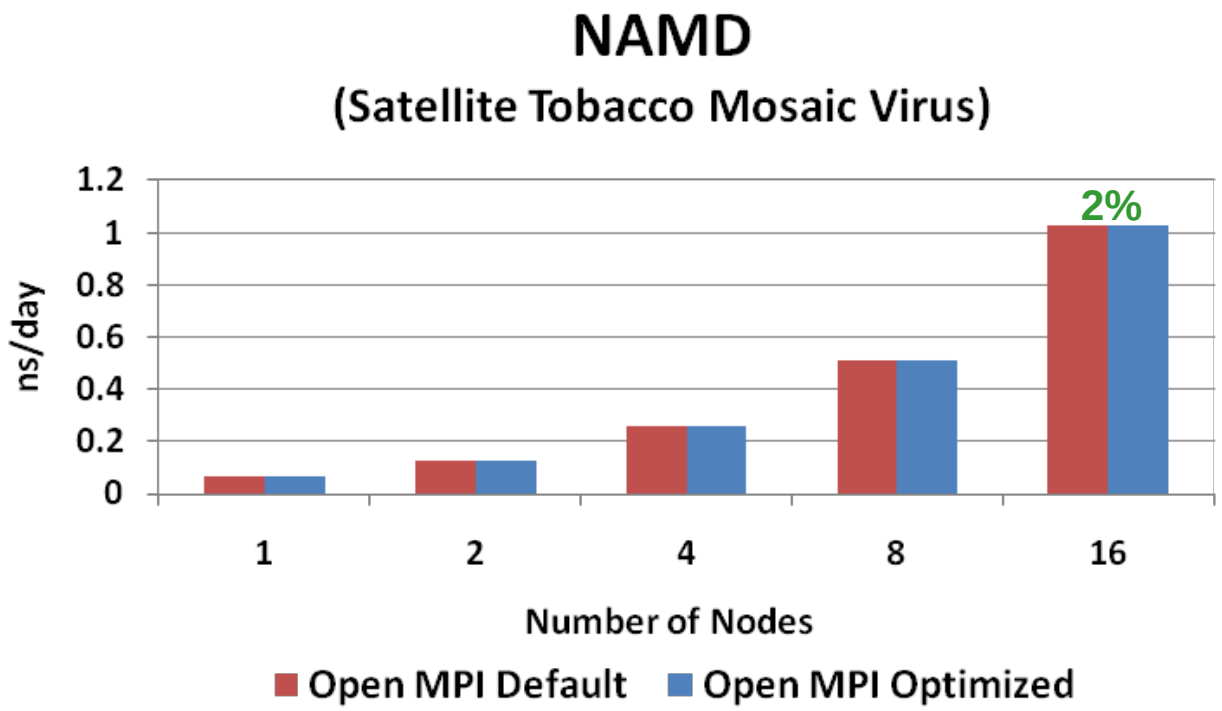


Higher is better

12 Cores/Node

NAMD Performance - Open MPI

- **Performance doesn't change much with different Rendezvous value**
  - 2% performance gain compared to default mode

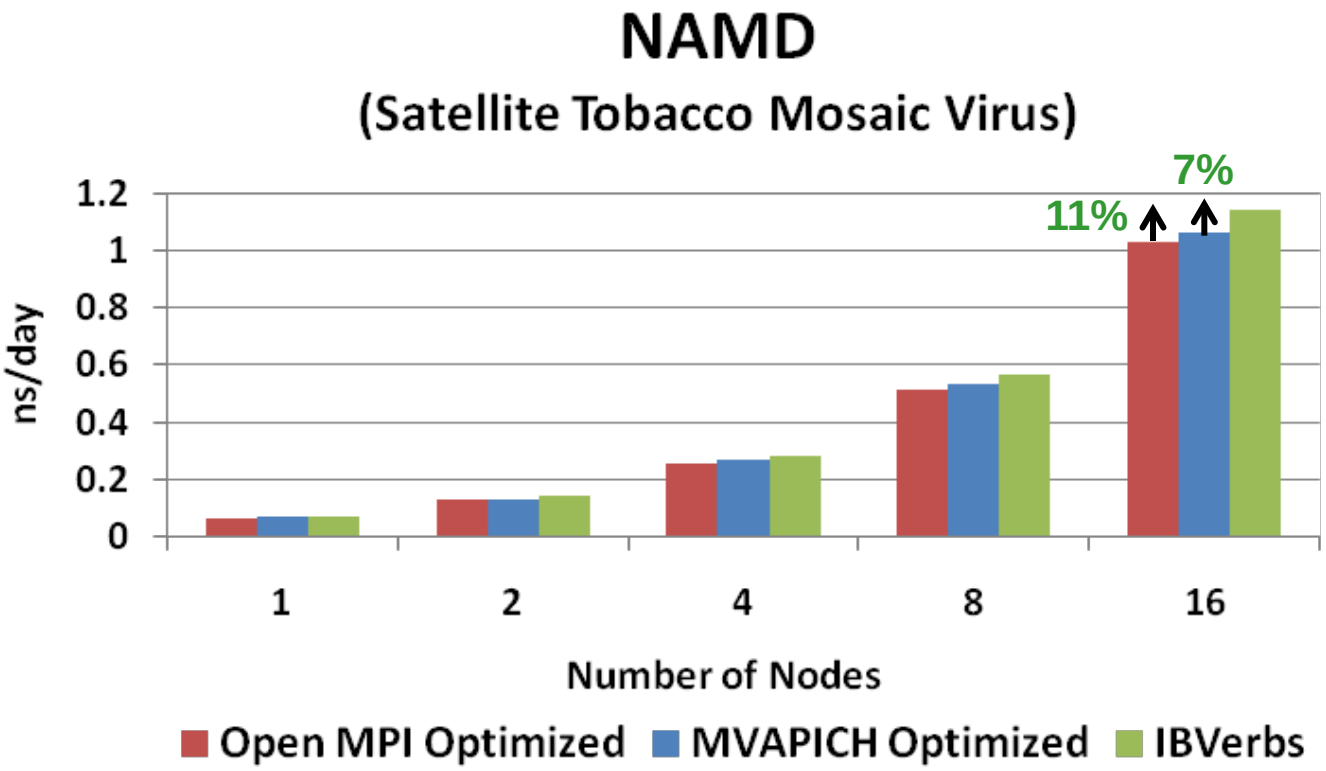


Higher is better

12 Cores/Node

NAMD Performance - IBverbs

- **Native IBverbs enables highest performance**
  - 11% higher than Open MPI and 7% higher than optimized MVAPICH at 16 nodes
  - Performance advantage increases as cluster scales

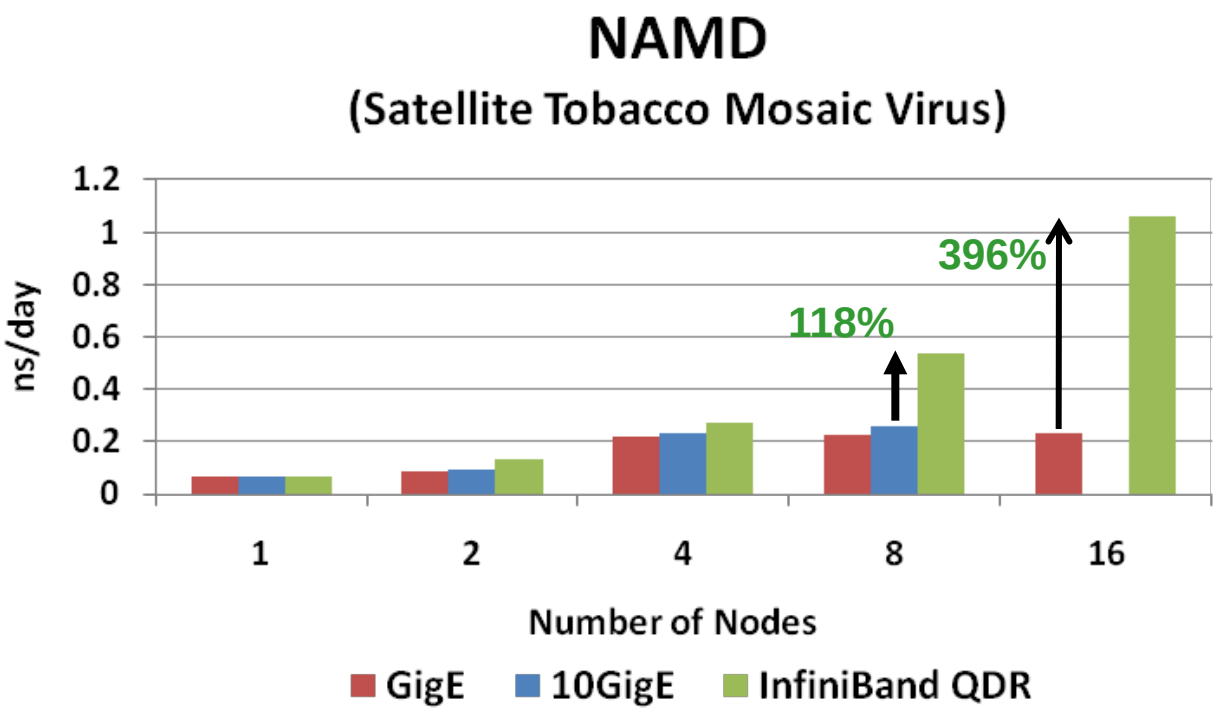


Higher is better

12 Cores/Node

NAMD Performance - Interconnect

- **InfiniBand QDR enables linear scalability**
  - 396% higher performance than GigE at 16 nodes
  - 118% higher performance than 10GigE at 8 nodes
  - Performance advantage extends as cluster size increases
- **InfiniBand reduces electrical energy/job**
  - by 80% or more compared to GigE
  - by 54% or more compared to 10GigE

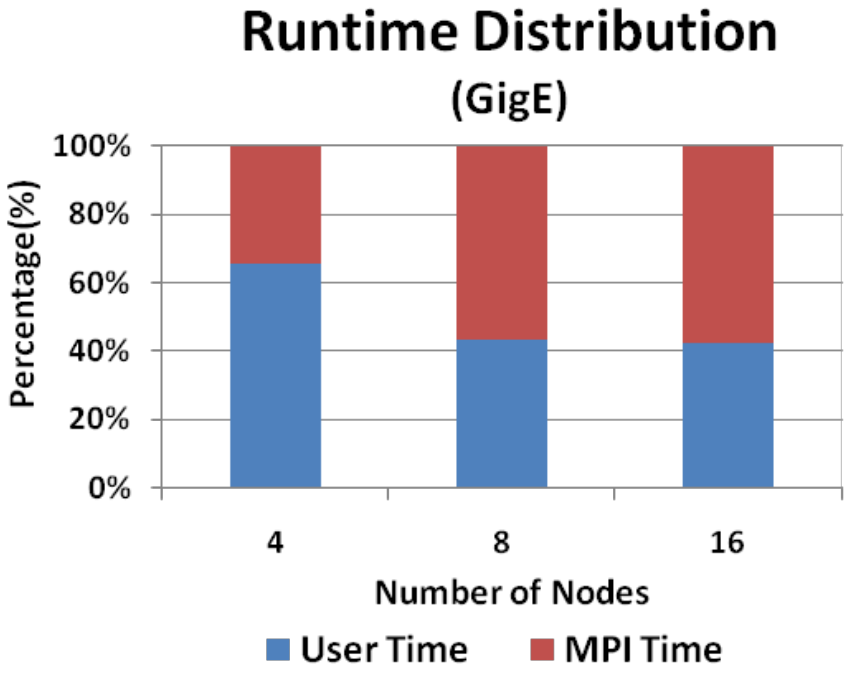


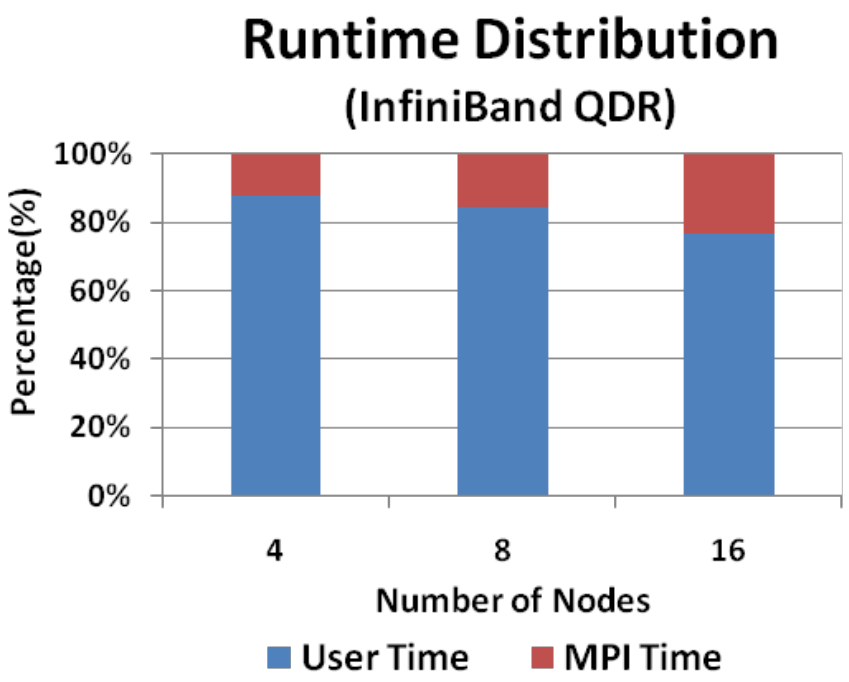
Higher is better

12 Cores/Node

NAMD MPI Profiling - Runtime Distribution

- **Runtime Distribution**
  - MPI overhead becomes dominated with GigE as node count increases
  - InfiniBand enables much smaller MPI communication overhead comparing to GigE

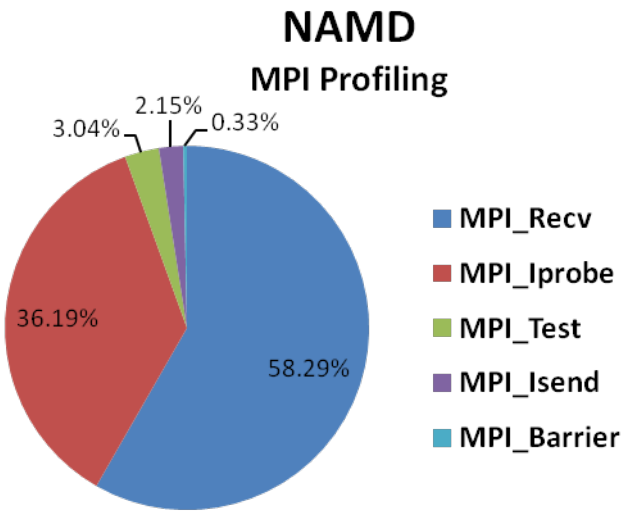




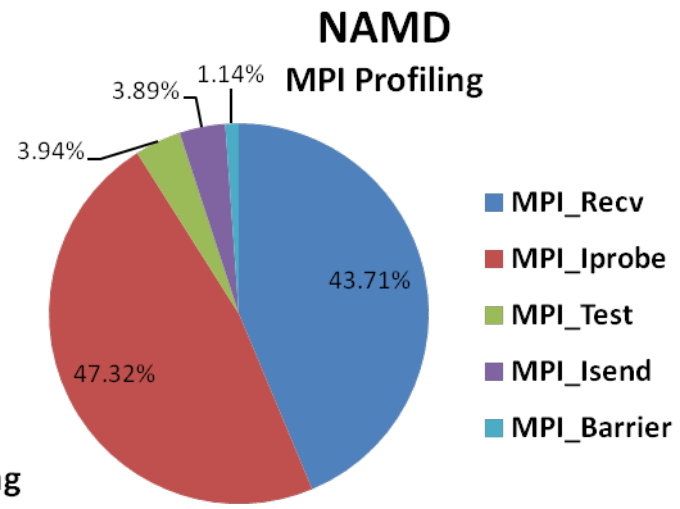
12 Cores/Node

NAMD MPI Profiling - MPI Overhead

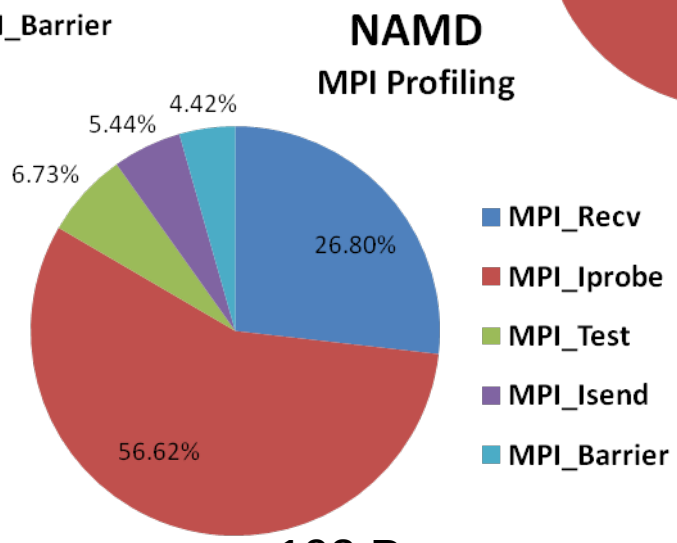
- **Mostly used MPI functions**
  - MPI_Iprobe and MPI_Recv create large overhead
  - MPI_Iprobe overhead increases faster than others as cluster size scales



48 Proceses



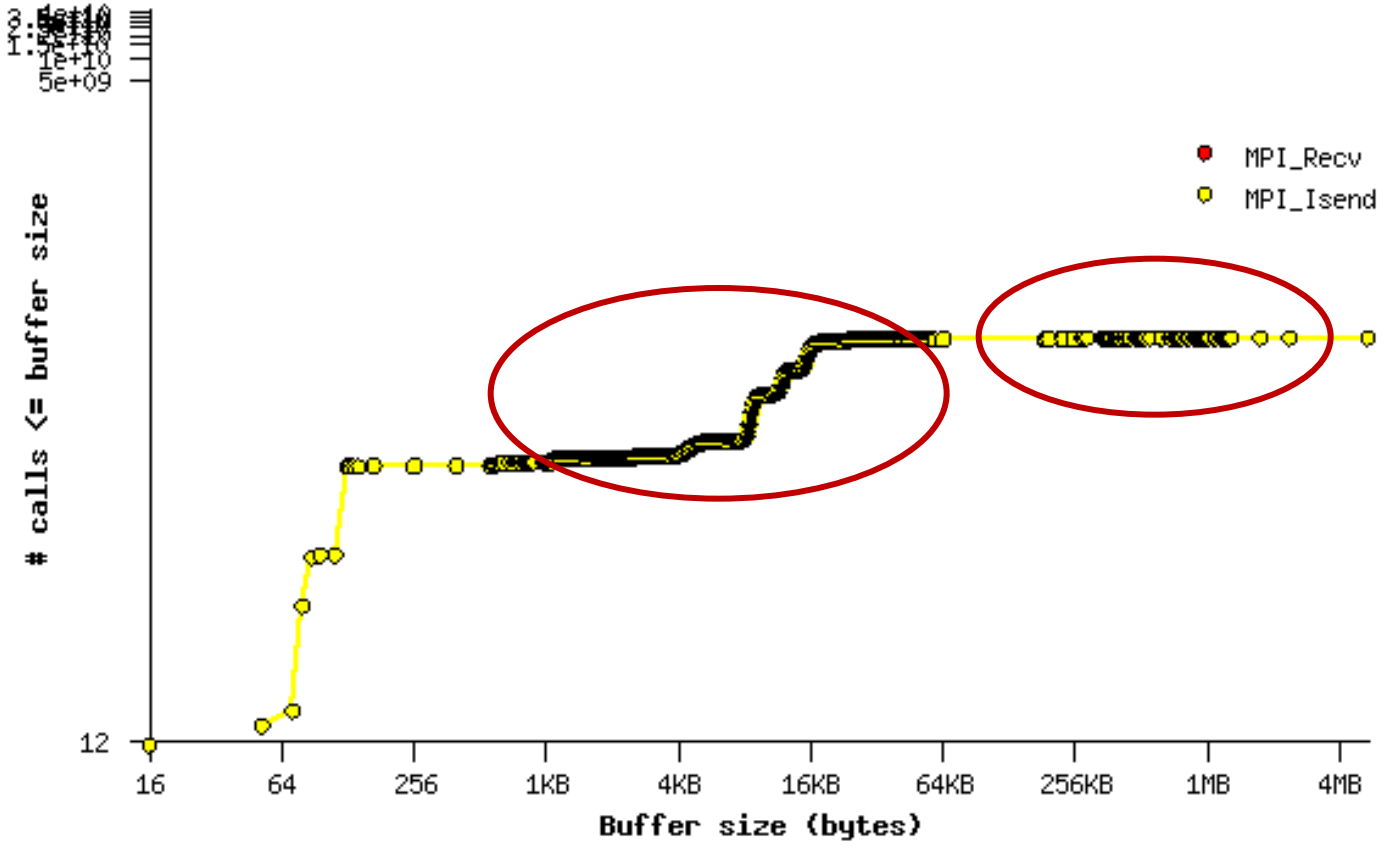
96 Processes



192 Processes

NAMD MPI Profiling - MPI Message Size

- **Most message size**
  - 512Bytes to 64KB, and 256KB to 2MB



NAMD Benchmark Summary

- **Interconnect comparison shows**
  - InfiniBand delivers superior performance in every cluster size
  - Low latency InfiniBand enables much higher scalability than10GigE and GigE
- **Communication libraries comparison shows**
  - MVAPICH tuning enables 11% higher performance than default setting
  - Native IBverbs delivers 7% or higher performance than MPI library
  - Performance gains further in both cases as cluster size grows
- **InfiniBand QDR saves power**
  - Reduces power consumption/job by
    - 80% comparing to GigE at 16 nodes (more saving expected at higher node count)
    - 54% comparing to 10GigE at 8 nodes (more saving expected at higher node count)
- **MPI Profiling shows both interconnect bandwidth and latency are important to enable NAMD performance and scalability**

Thank You

HPC Advisory Council