NETWORK OF EXPERTISE

CPMD Performance Benchmark, Profiling and Tuning

November 2010

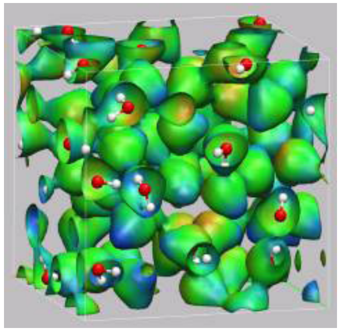
Note

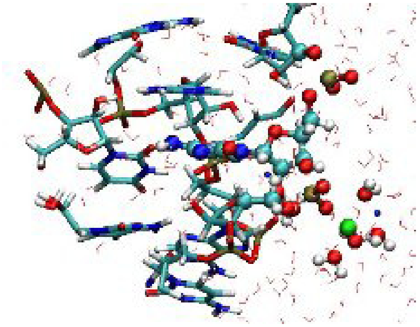
- **The following research was performed under the HPC Advisory Council activities**
  - Participating vendors: Intel, Dell, Mellanox
  - Compute resource - HPC Advisory Council Cluster Center

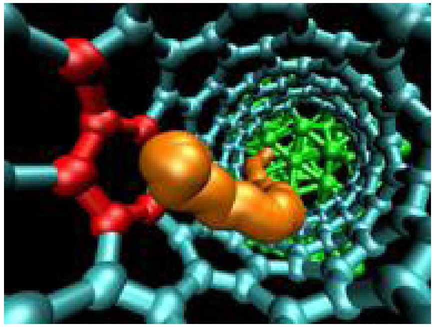
- **For more info please refer to**
  - http://www.dell.com
  - http://www.intel.com
  - http://www.mellanox.com
  - http://www.cpmd.org

Car-Parrinello Molecular Dynamics (CPMD)

- **CPMD**
  - A parallelized implementation of density functional theory (DFT)
  - Particularly designed for ab-initio molecular dynamics
  - Brings together methods
    - Classical molecular dynamics
    - Solid state physics
    - Quantum chemistry
- **CPMD supports MPI and Mixed MPI/SMP**
- **CPMD is distributed and developed by the CPMD consortium**







Objectives

- **The following was done to provide best practices**
  - – CPMD performance benchmarking
  - – Interconnect performance comparisons
  - – Understanding CPMD communication patterns
  - – Power-efficient simulations

- **The presented results will demonstrate**
  - – The scalability of the compute environment to provide nearly linear application scalability
  - – The capability of CPMD to achieve scalable productivity
  - – Considerations for power saving through balanced system configuration

Test Cluster Configuration

- **Dell™ PowerEdge™ M610 14-node cluster**
  - Six-Core Intel X5670 @ 2.93 GHz CPUs
  - Memory: 24GB memory, DDR3 1333 MHz
  - OS: CentOS5U4, OFED 1.5.1 InfiniBand SW stack
- **Intel Cluster Ready certified cluster**
- **Mellanox ConnectX-2 InfiniBand adapters and switches**
- **MPI: Intel MPI 4.0 U1, Open MPI 1.5, Platform MPI 8.0.1**
- **Compilers: GNU Compilers 4.1.2, Intel Compilers 12.0.0**
- **Math Libraries: ATLAS 3.8.3, BLAS 3.0.8, LAPACK, FFTW 2.1.5, MKL 10.3**
- **Application: CPMD 3.13.2_01**
- **Benchmark: Si512 Inp-1**

About Intel® Cluster Ready

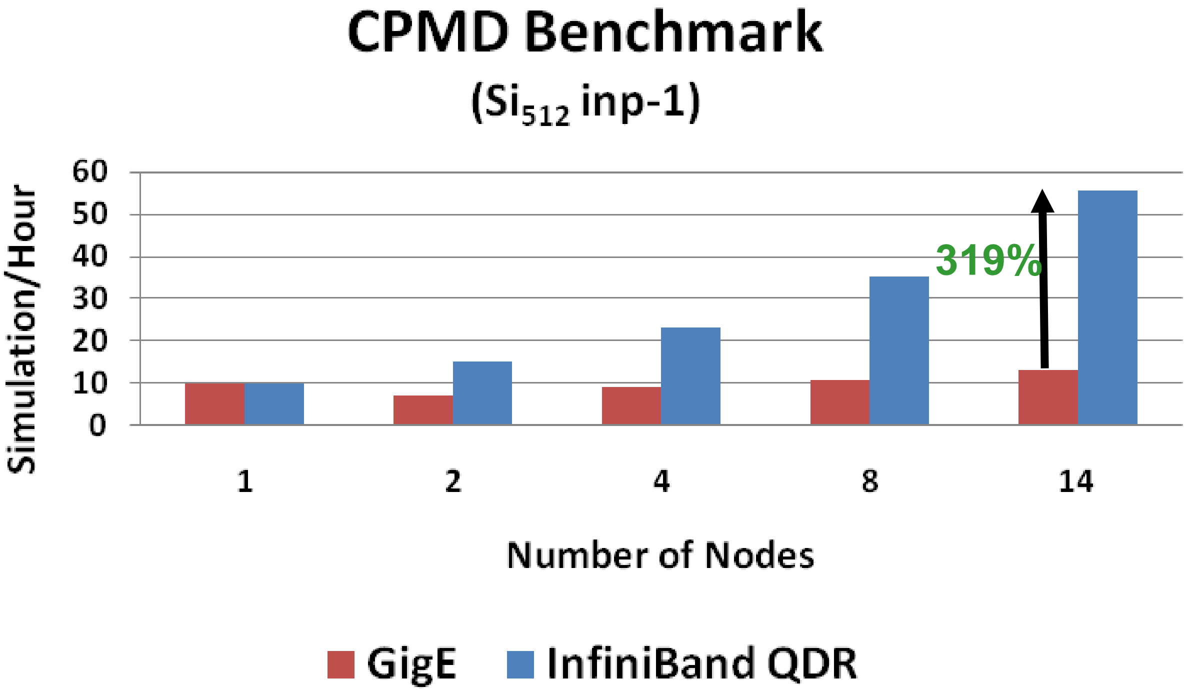
- **Intel® Cluster Ready systems make it practical to use a cluster to increase your simulation and modeling productivity**
  - Simplifies selection, deployment, and operation of a cluster
- **A single architecture platform supported by many OEMs, ISVs, cluster provisioning vendors, and interconnect providers**
  - Focus on your work productivity, spend less management time on the cluster
- **Select Intel Cluster Ready**
  - Where the cluster is delivered ready to run
  - Hardware and software are integrated and configured together
  - Applications are registered, validating execution on the Intel Cluster Ready architecture
  - Includes Intel® Cluster Checker tool, to verify functionality and periodically check cluster health

Dell PowerEdge Servers helping Simplify IT

- **System Structure and Sizing Guidelines**
  - 14-node cluster build with Dell PowerEdge™ M610 blades server
  - 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

CPMD Performance – Interconnect

- **InfiniBand enables higher scalability**
  - Up to 319% higher performance than Ethernet at 14 nodes
- **Ethernet would not scale beyond 1 node**
  - Show virtually no gain by increasing nodes

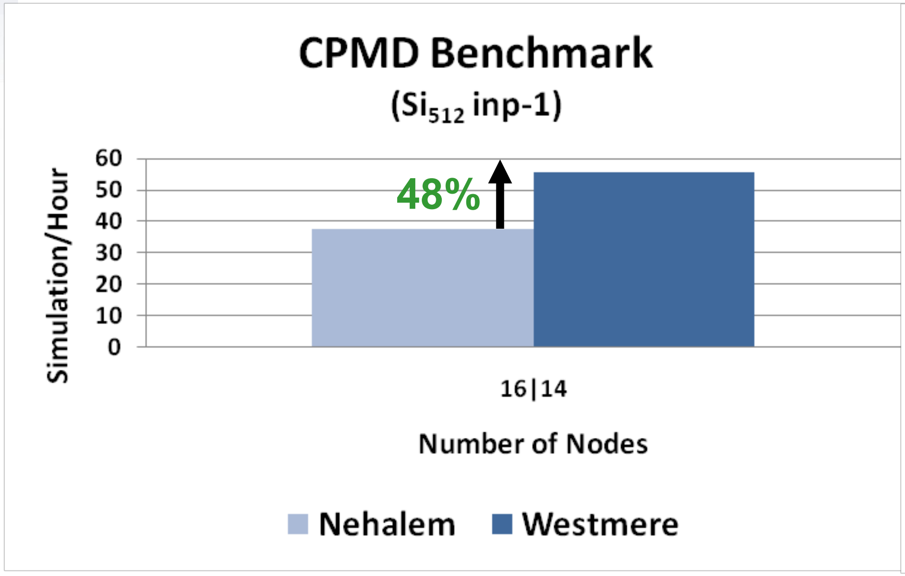


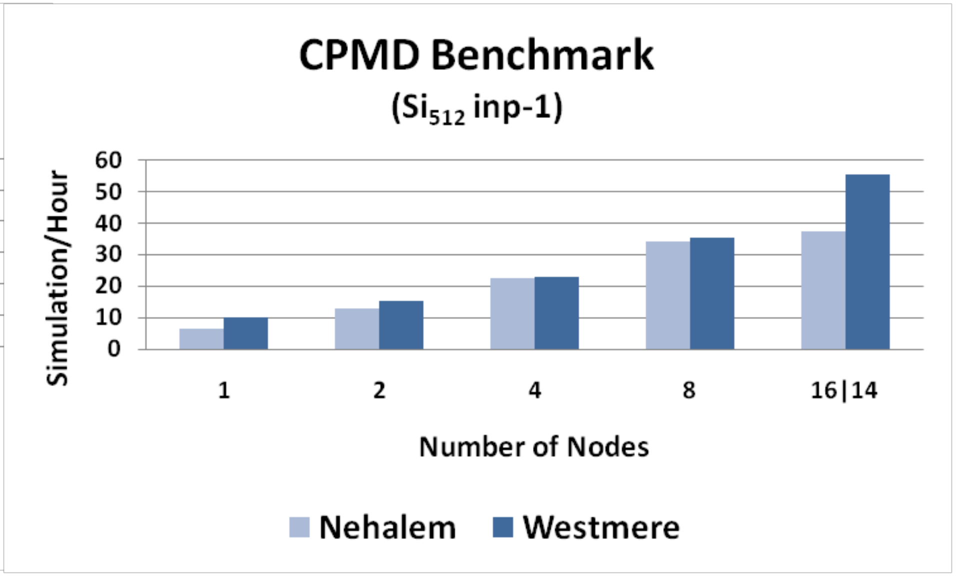
Higher is better

12 Cores/Node

CPMD Performance – Nehalem vs Westmere

- **Westmere processors enabled better performance**
  - Up to 48% gain with 14 Westmere node compared to 16 Nehalem nodes



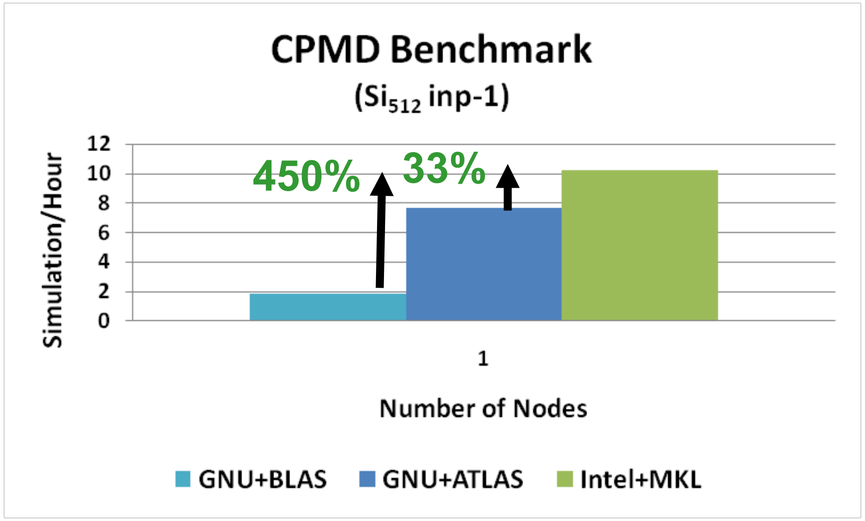


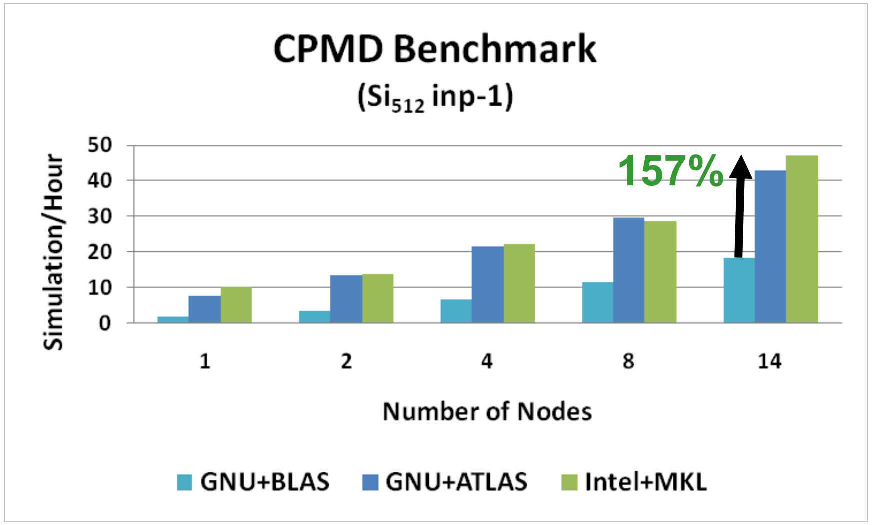
Higher is better

12 Cores/Node

CPMD Performance – Compilers and Libraries

- **Intel compilers and MKL enable the best performance**
  - Up to 450% gain on a single node versus GNU compilers with the BLAS libraries
  - Up to 33% gain on a single node versus GNU compilers with the ATLAS libraries
- **ATLAS can be a good alternative to BLAS**
  - ATLAS (Automatically Tuned Linear Algebra Software)





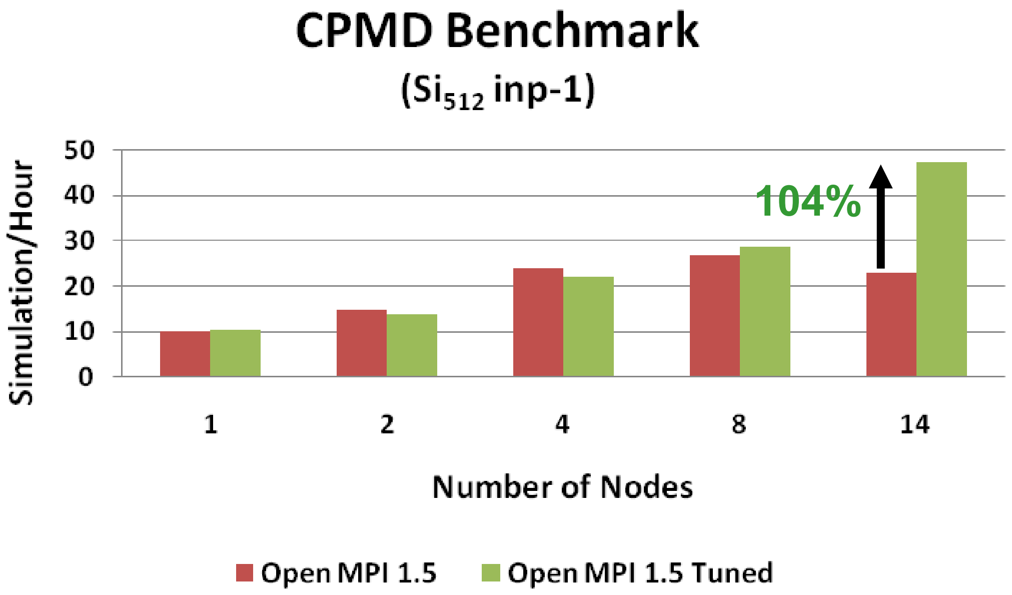
Open MPI 1.5

12 Cores/Node

Higher is better

CPMD Performance – Open MPI Tuning

- **Selecting tuned collectives algorithms can provide boost performance**
  - Up to 104% in performance improvement
  - The difference is more apparent on larger number of nodes or processes
  - Tuning MPI_Alltoall and MPI_Allreduce can make a positive impact
- **Optimize Open MPI using the following MCA parameters**
  - coll_tuned_use_dynamic_rules 1, coll_tuned_alltoall_algorithm 3, coll_tuned_allreduce_algorithm 4, mpi_paffinity_alone 1

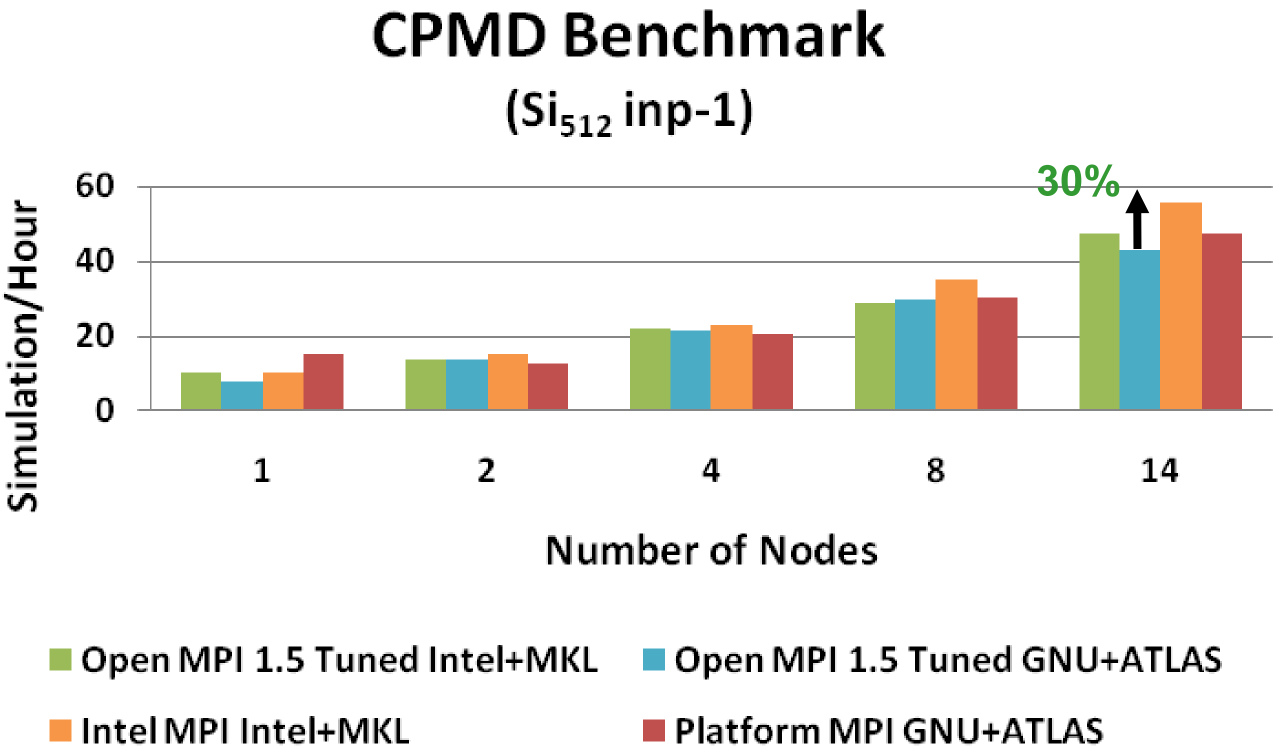


Higher is better

12 Cores/Node

CPMD Performance – MPI

- **Intel MPI shows better scalability over the tuned Open MPI**
  - Shows 30% gain over tuned Open MPI with GNU compilers and ATLAS

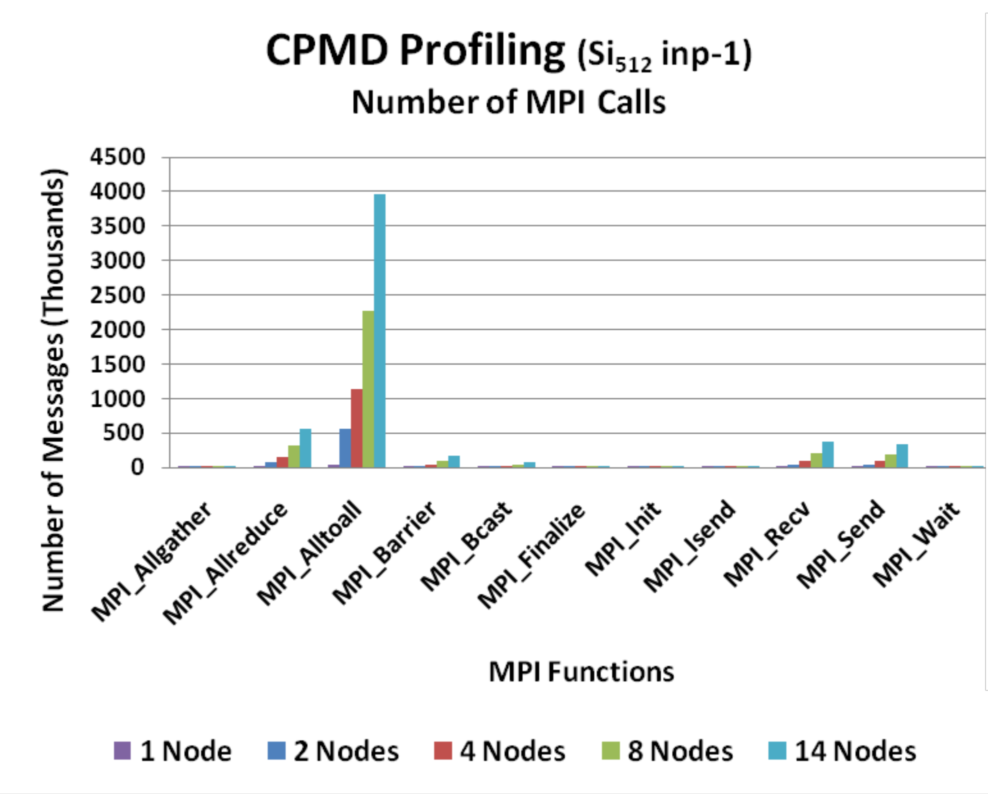


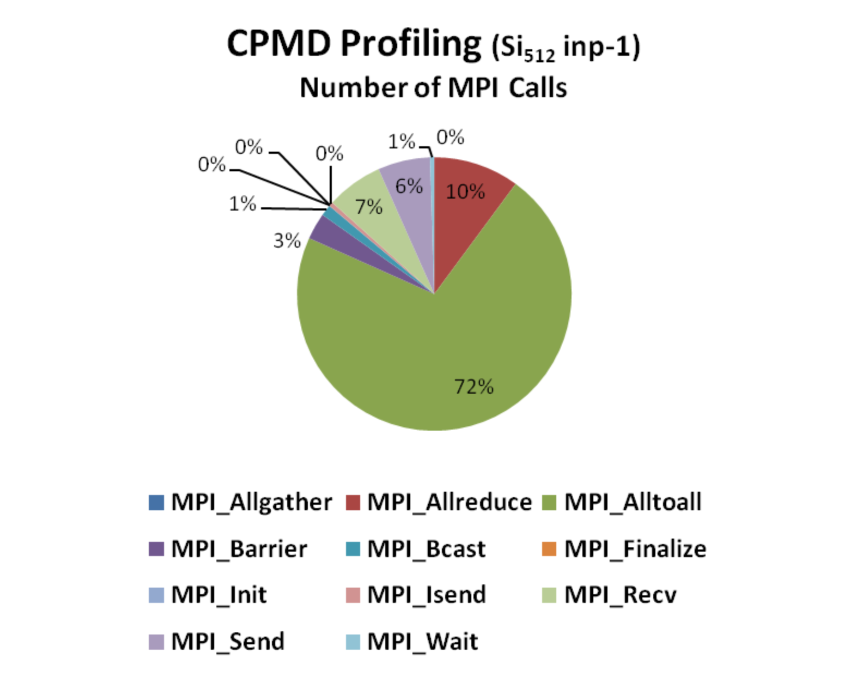
Higher is better

12 Cores/Node

CPMD Profiling – Number of MPI Calls

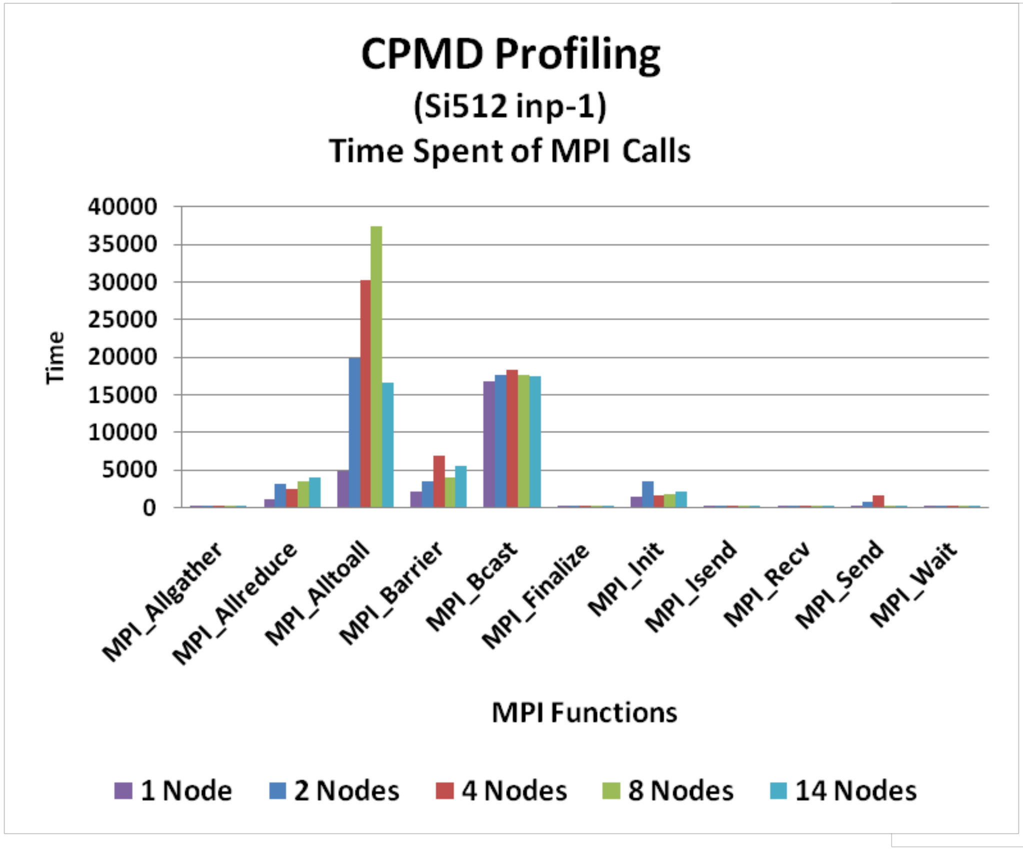
- **The most used MPI functions with this dataset is MPI_Alltoall**
- **MPI_Alltoall accounted for 72% of all MPI calls on a 14-node job**

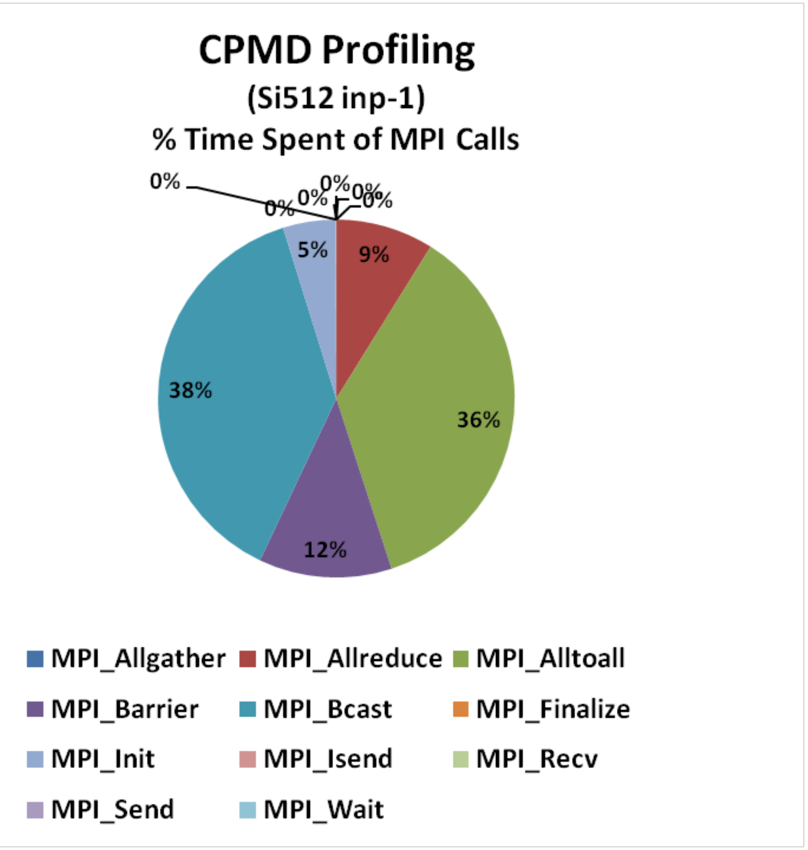




CPMD Profiling – Time Spent of by MPI Calls

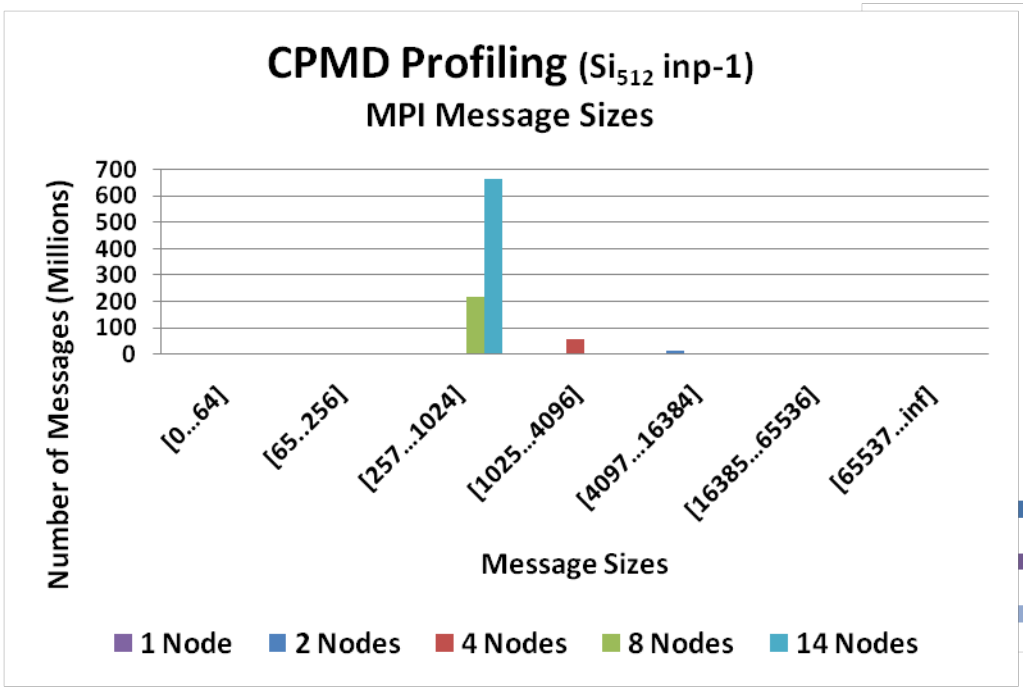
- **Majority of time is spent on MPI_Alltoall and MPI_Bcast**
  - MPI_Alltoall is accounted for 38% of time spent on a 14-node job
  - MPI_Bcast is accounted for 36% of time spent on a 14-node job

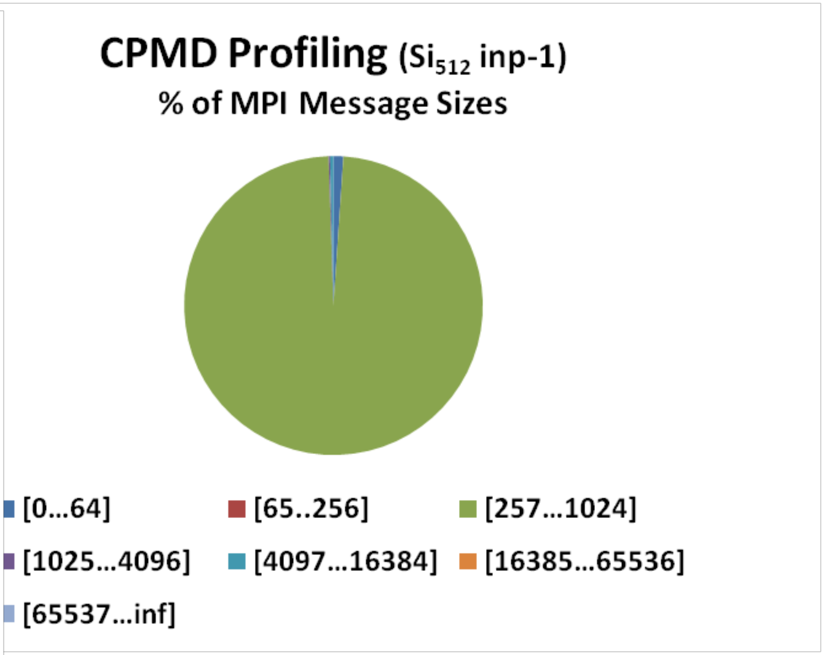




CPMD Profiling – MPI Message Sizes

- **Majority of messages are small messages**
  - Messages between 256B and 1KB are the majority for the 14-node and 8-node runs
  - Accounted for 98% of the MPI message sizes on the 14 nodes





Summary

- **Interconnects effect to CPMD performance**
  - InfiniBand enables higher performance/scalability
  - Up to 319% higher performance than Ethernet at 14 nodes
- **Intel Westmere processor delivers better performance**
  - Up to 48% gain on a 14-node Westmere processors versus 16-node on Nehalem processors
- **Intel compilers and MKL provides better performance**
  - Up to 450% gain on a single node over GNU compilers with BLAS
  - Up to 33% gain on a single node over GNU compilers with ATLAS
- **Intel MPI shows better scalability over the tuned Open MPI**
- **Tuning MPI_Alltoall and MPI_Allreduce provide up to 104% improvement for Open MPI**
- **Majority of MPI messages are between 256B and 1KB**
- **MPI_Alltoall is the most used MPI functions**
- **Majority of MPI time is spent on MPI_Alltoall and MPI_Bcast**

Thank You

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