HPC
ADVISORY COUNCIL

PARATEC Performance Benchmark and Profiling

April 2010

AMD
The future is fusion

DELL

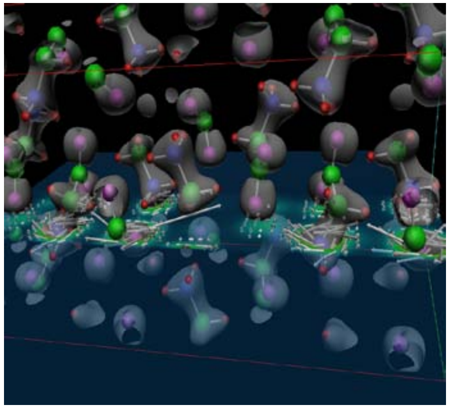
Mellanox
TECHNOLOGIES

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**
  - www.mellanox.com, www.dell.com/hpc, www.amd.com
  - http://www.nersc.gov/projects/paratec/

PARATEC

- PARATEC stands for PARAllel Total Energy Code
- Performs ab-initio quantum-mechanical total energy calculations using pseudopotentials and a plane wave basis set
- Designed to run on massively parallel computing platforms and clusters
- Developed through a joint collaboration between
  - LBNL
  - Université Pierre et Marie CURIE
  - University of Montreal
  - University of Cambridge



Objectives

- **The presented research was done to provide best practices**
  - PARATEC performance benchmarking
    - Performance tuning with different communication libraries and compilers
    - Interconnect performance comparisons
  - Understanding PARATEC communication patterns
  - Power-efficient simulations
- **The presented results will demonstrate**
  - Balanced compute system enables
    - Good application scalability
    - Power saving

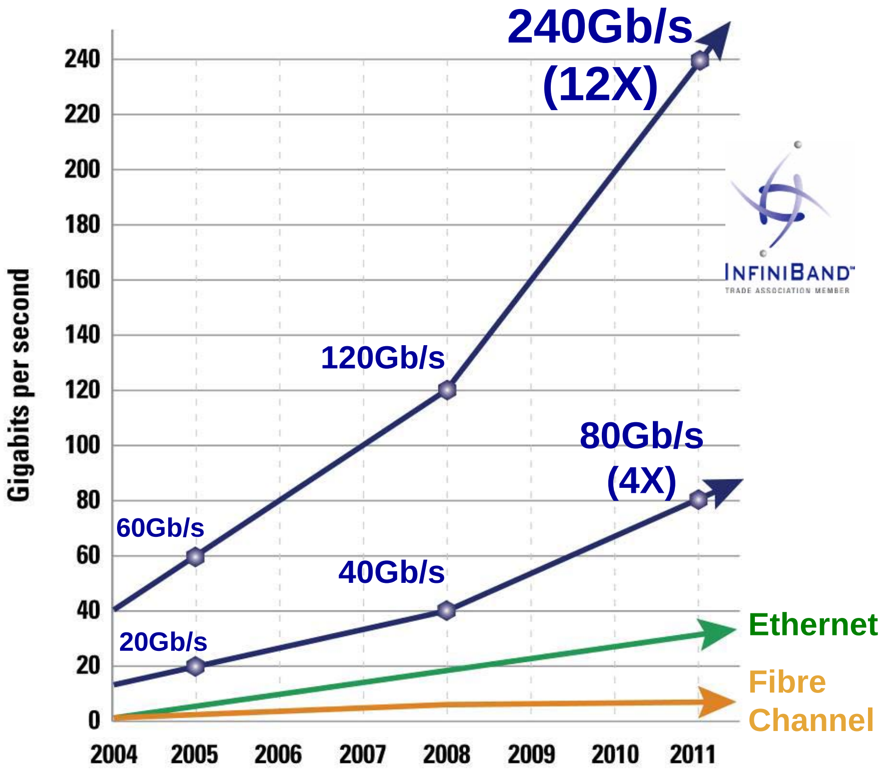
Test Cluster Configuration

- **Dell™ PowerEdge™ SC 1435 16-node cluster**
- **Quad-Core AMD Opteron™ 2382 (“Shanghai”) CPUs**
- **Mellanox® InfiniBand ConnectX® 20Gb/s (DDR) HCAs**
- **Mellanox® InfiniBand DDR Switch**
- **Memory: 16GB memory, DDR2 800MHz per node**
- **OS: RHEL5U3, OFED 1.5 InfiniBand SW stack**
- **Compiler and Math library: Intel compiler 11.1, Intel MKL 11.1**
- **MPI: OpenMPI-1.3.3, Intel MPI 4.0**
- **Application: PARATEC**
- **Benchmark Workload**
  - Large size
    - Silicon in diamond (343 atoms)

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**

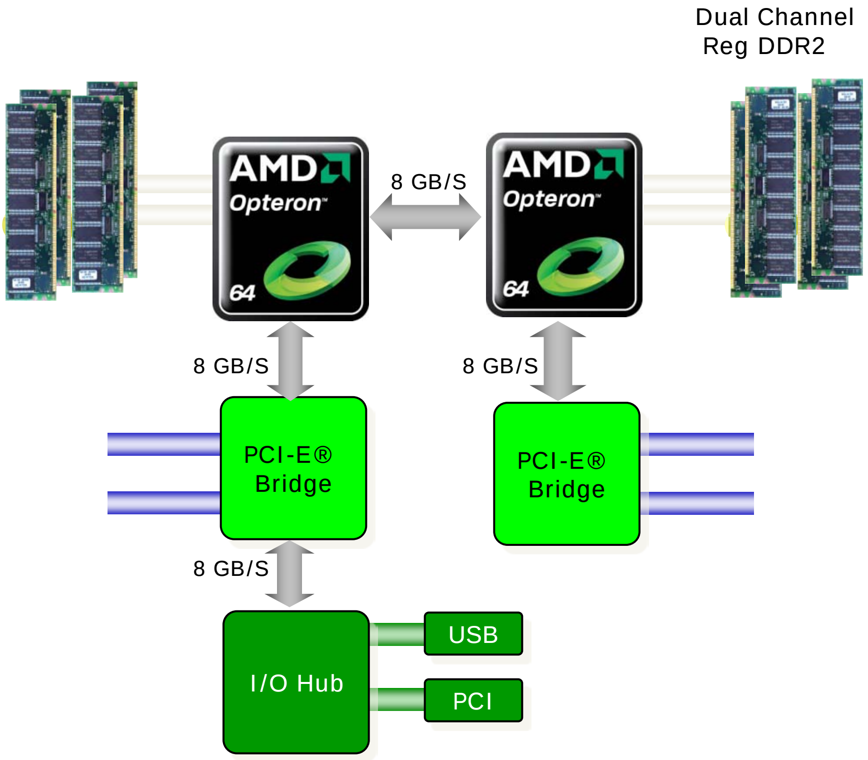
The InfiniBand Performance Gap is Increasing



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/clk 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 2nd / 3rd generation AMD Opteron™ processor

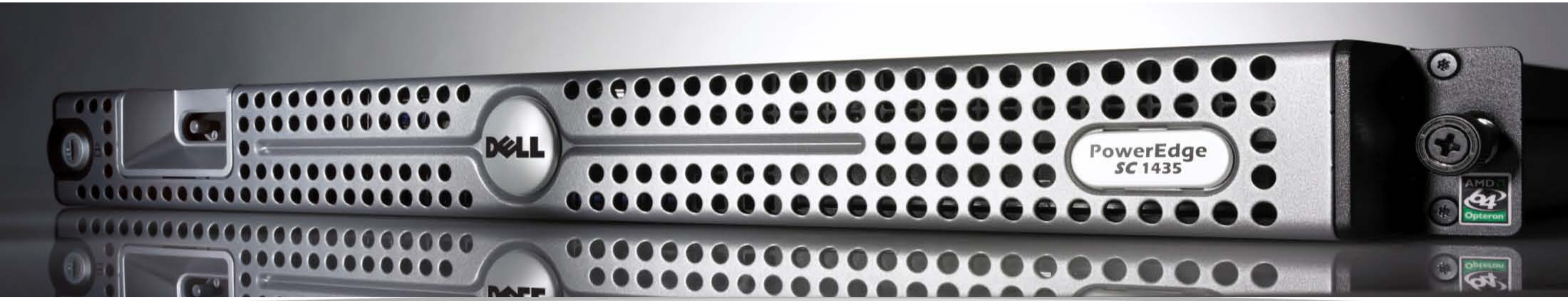


Dell PowerEdge Servers helping Simplify IT

- **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

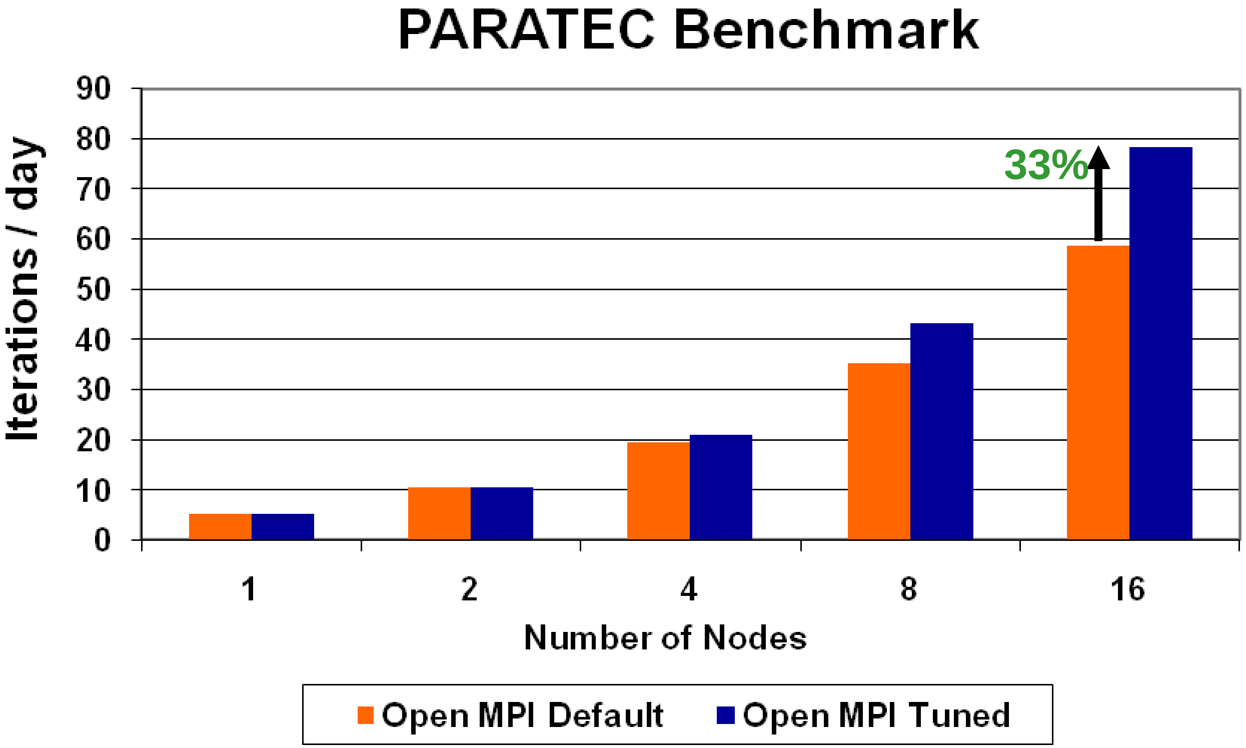
Dell PowerEdge™ Server Advantage

- Dell™ PowerEdge™ servers incorporate AMD Opteron™ and Mellanox ConnectX InfiniBand to provide leading edge performance and reliability
- Building Block Foundations for best price/performance and performance/watt
- Investment protection and energy efficient
- Longer term server investment value
- Faster DDR2-800 memory
- Enhanced AMD PowerNow!
- Independent Dynamic Core Technology
- AMD CoolCore™ and Smart Fetch Technology
- Mellanox InfiniBand end-to-end for highest networking performance



PARATEC Benchmark Results

- **Optimized MPI parameter provide better performance**
  - **Up to 33% higher performance with customized MPI_Gather, barrier, and XRC parameter**
    - --mca btl_openib_receive_queues X,9216,256,128,32:X,65536,256,128,32 --mca coll_tuned_use_dynamic_rules 1 --mca coll_tuned_gather_algorithm 1 --mca coll_tuned_barrier_algorithm 3

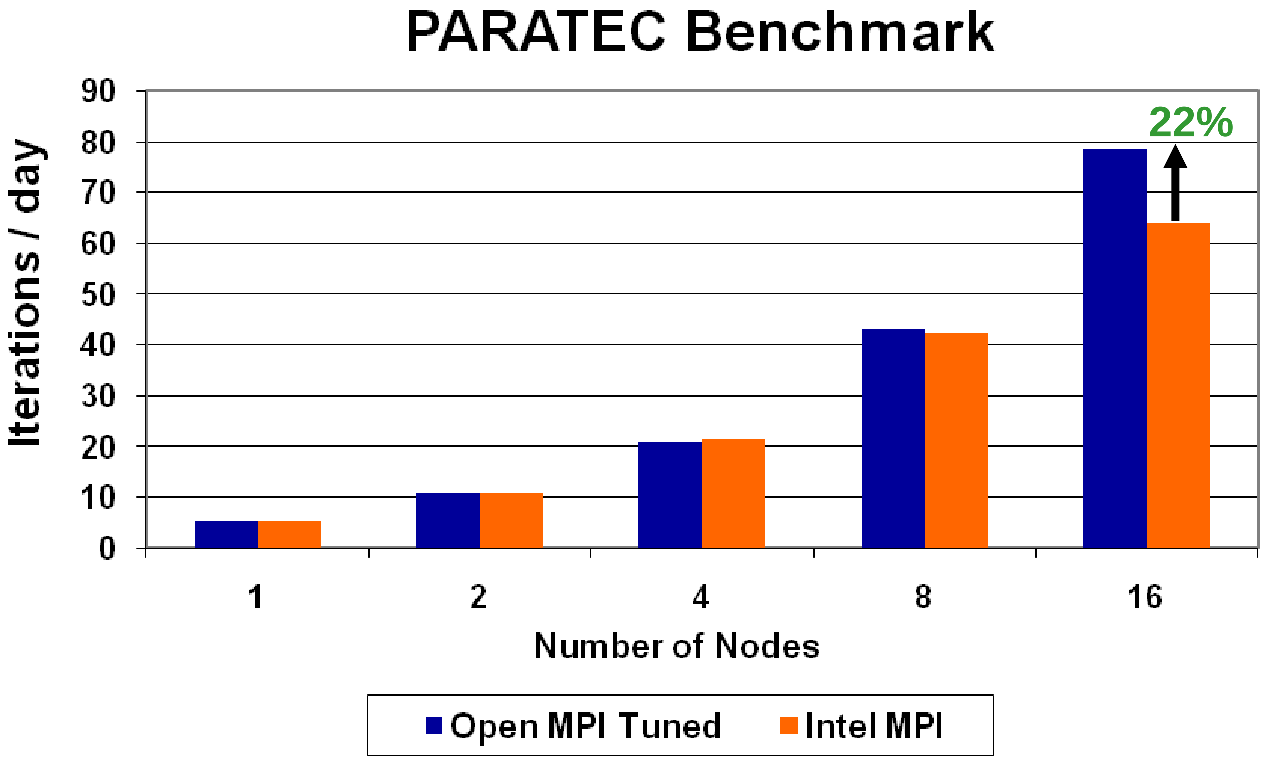


Higher is better

8-cores per node

PARATEC Benchmark Results

- **Open MPI with optimization enables higher performance**
  - Up to 22% higher performance than Intel MPI

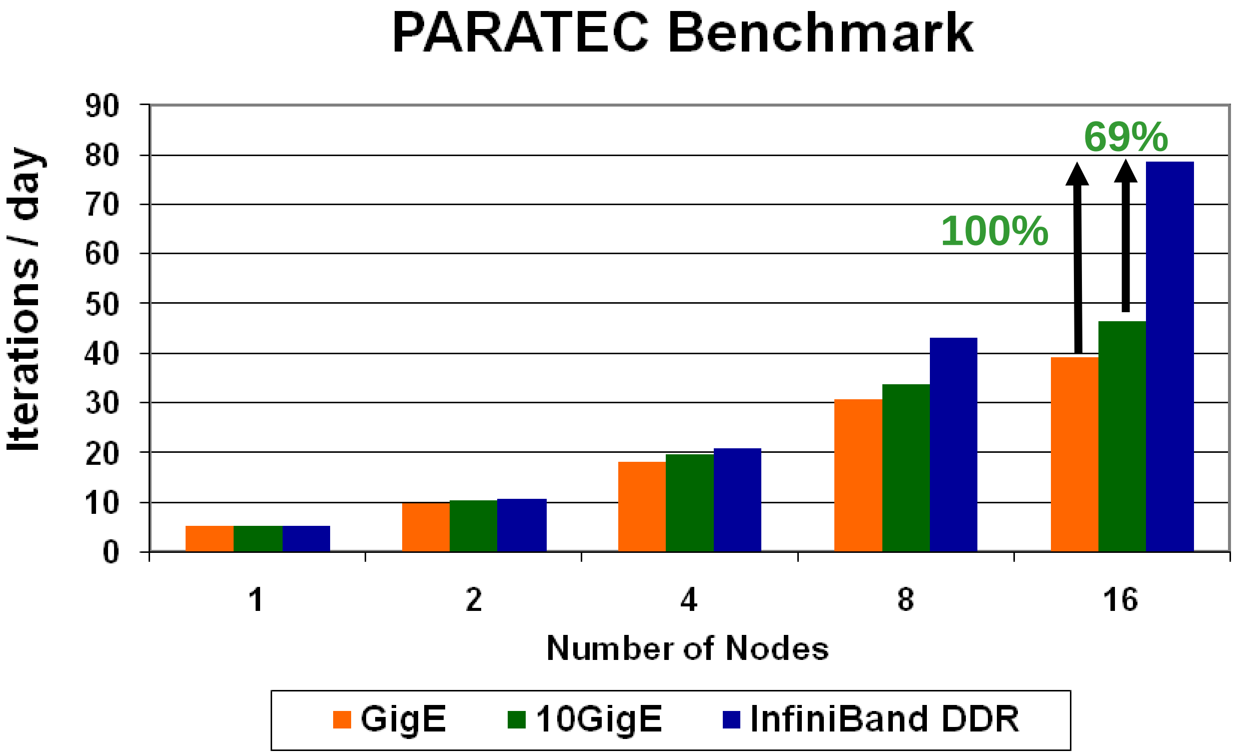


Higher is better

8-cores per node

PARATEC Benchmark Results

- **InfiniBand enables better application performance and scalability**
  - Up to 69% higher performance than 10GigE and 100% than GigE
  - 16-node cluster
- **Application performance over InfiniBand scales as cluster size increases**

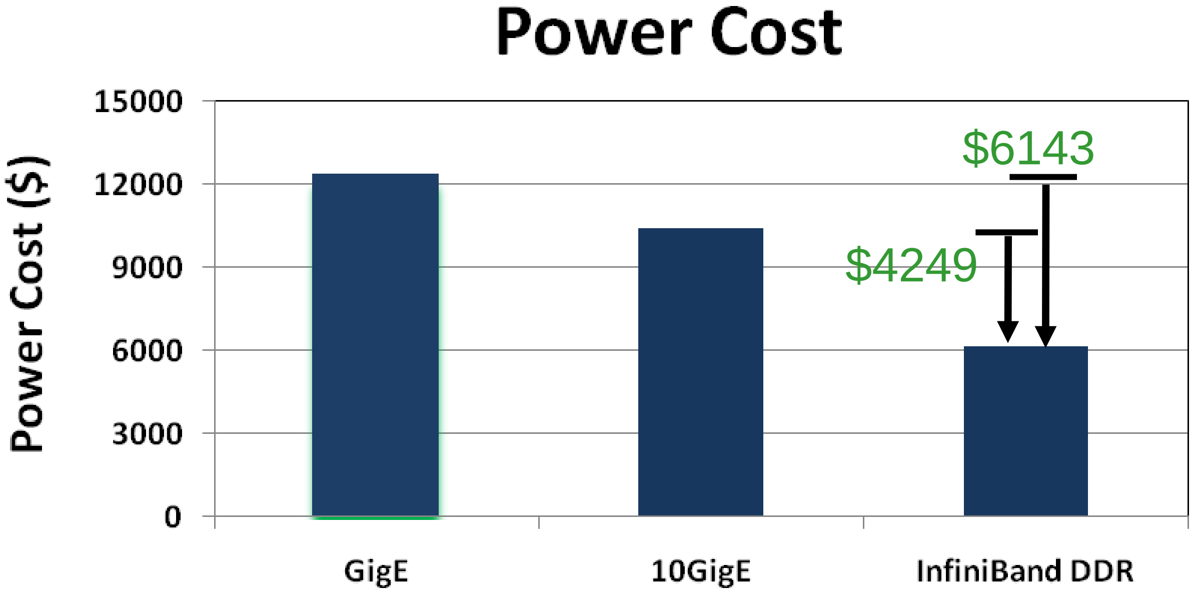


Higher is better

8-cores per node

Power Cost Savings with Different Interconnect

- **Dell economical integration of AMD CPUs and Mellanox InfiniBand**
  - To achieve same number of PARATEC jobs over GigE
  - InfiniBand saves power up to $4249 versus 10GigE and $6143 versus GigE
  - Yearly based for 16-node cluster
- **As cluster size increases, more power can be saved**



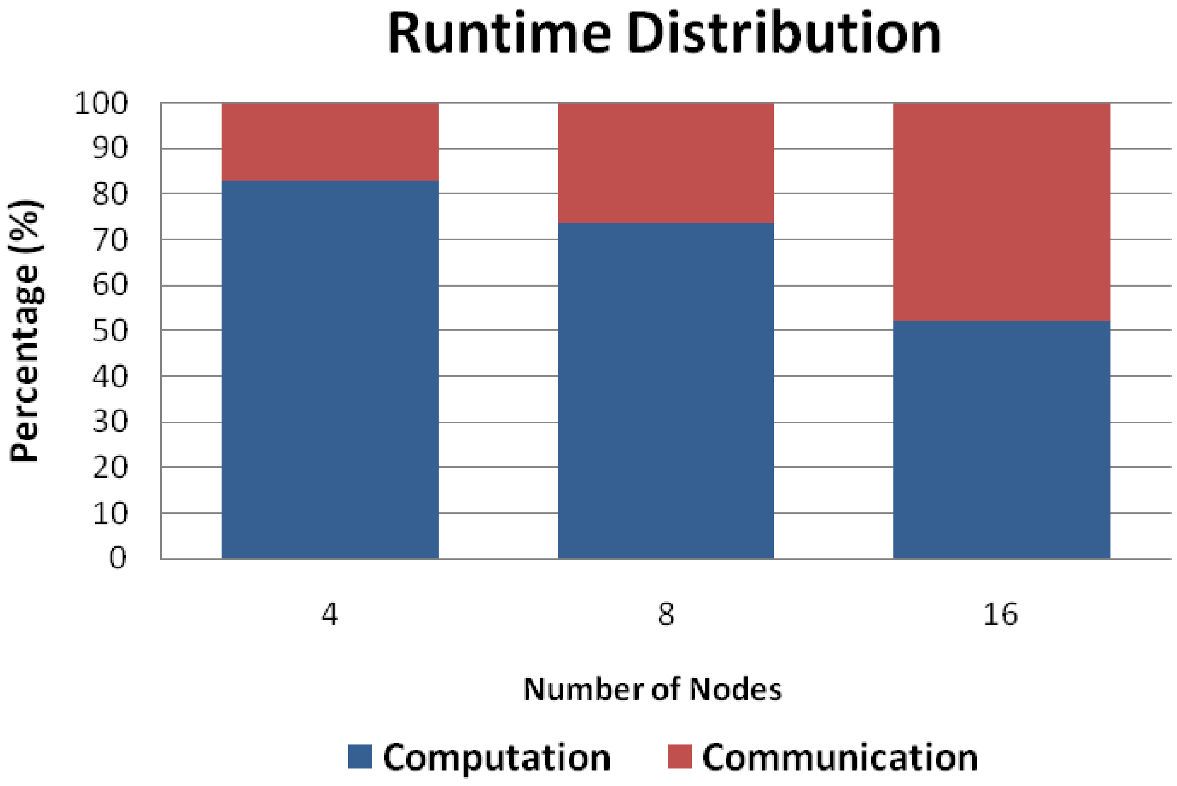
*$/KWh = KWh * $0.20*
For more information - http://enterprise.amd.com/Downloads/svrpwrusecompletefinal.pdf

PARATEC Benchmark Summary

- **Tuned MPI parameters provides better performance**
  - – Customized MPI collectives and XRC algorithm can improve application performance by 33%
- **Interconnect comparison shows**
  - – InfiniBand delivers superior performance in every cluster size versus GigE and 10GigE
  - – Performance advantage extends as cluster size increases
- **InfiniBand enables power saving**
  - – Up to $6143/year power savings versus GigE and $4249 versus 10GigE on16 node cluster
- **Dell™ PowerEdge™ server blades provides**
  - – Linear scalability (maximum scalability) and balanced system
    - By integrating InfiniBand interconnect and AMD processors
  - – Maximum return on investment through efficiency and utilization

PARATEC MPI Profiling – Runtime Distribution

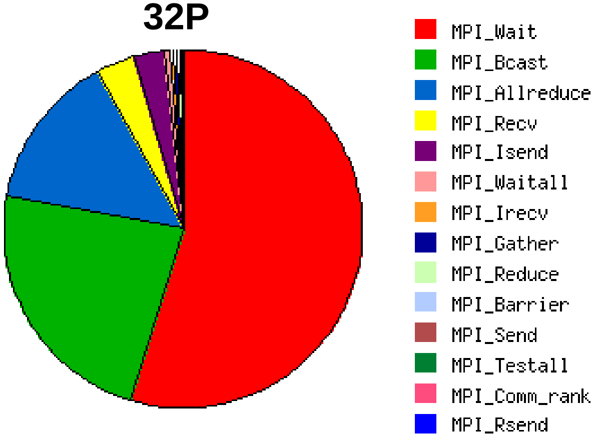
- **Mostly used MPI functions**
  - Percentage of communication increases as cluster size scales



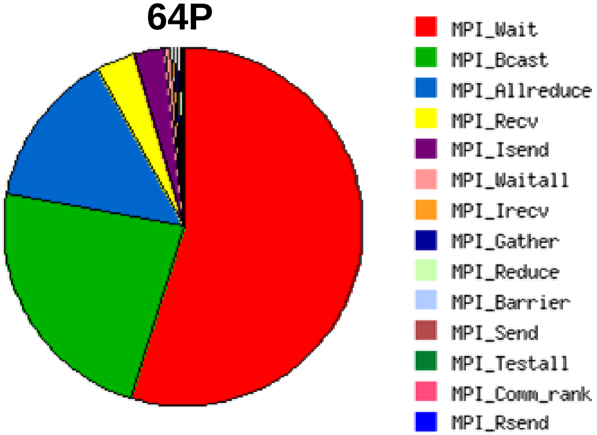
PARATEC MPI Profiling – MPI Functions

- **Mostly used MPI functions**
  - MPI_Wait, MPI_Allreduce, and MPI_Bcast are the mostly used MPI functions
  - MPI_Allreduce overhead becomes large when running processes is larger than 64

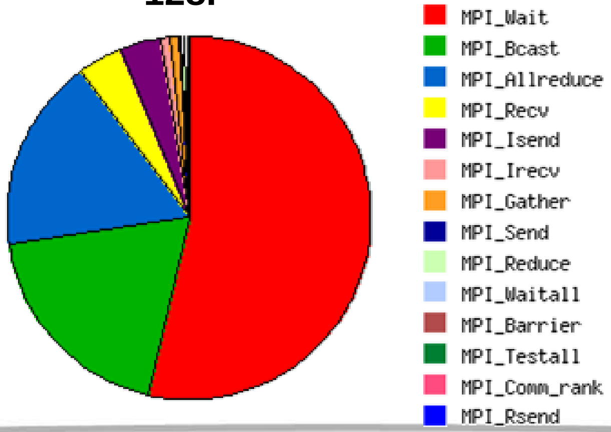
32P



64P

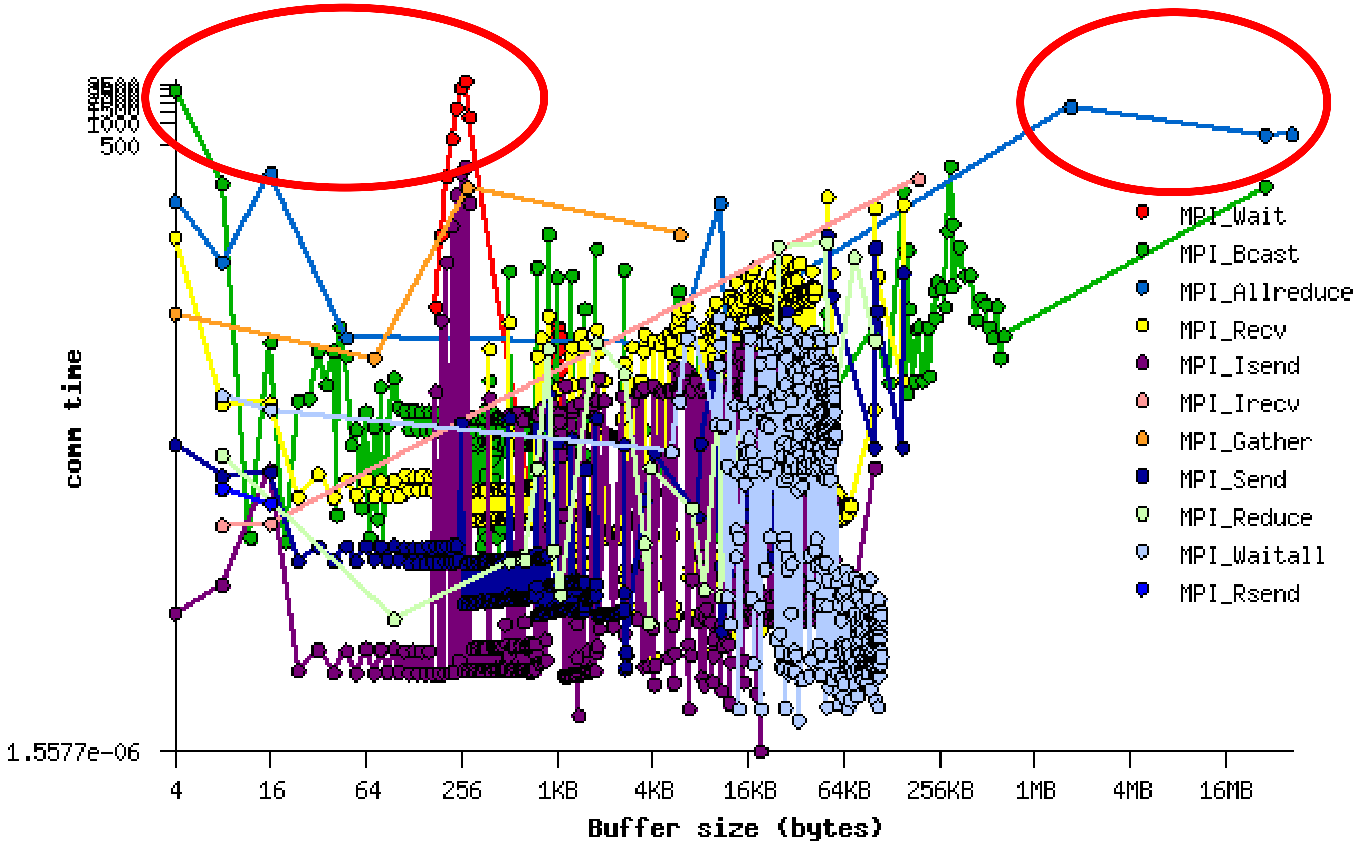


128P



PARATEC MPI Profiling – Message Size

- **Messages with big communication overhead are**
  - Large messages >1MB
  - Small message <256Bytes



128 Processes

PARATEC Profiling Summary

- **PARATEC was profiled to identify its communication patterns**
  - MPI collective and point-to-point create the big communication overhead
  - Both small and large messages are used
  - Number of messages increases with cluster size
- **Interconnects effect to PARATEC performance**
  - Latency and bandwidth are critical to application performance
- **Balanced system – CPU, memory, Interconnect that match each other capabilities, is essential for providing application efficiency**

Thank You

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