PARATEC Performance Benchmark and Profiling

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

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The InfiniBand Performance Gap is Increasing

- **240Gb/s** (12X)
- **120Gb/s**
- **80Gb/s** (4X)
- **60Gb/s**
- **40Gb/s**
- **20Gb/s**

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
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**

**PARATEC Benchmark**

- **Higher is better**

![Graph showing performance over InfiniBand as node count increases.](image)
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**

$\$/KWh = KWh \times 0.20$

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 on 16 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
• Mostly used MPI functions
  – Percentage of communication increases as cluster size scales
**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
• Messages with big communication overhead are
  - Large messages >1MB
  - Small message <256Bytes
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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