CP2K
Performance Benchmark and Profiling

April 2011
• The following research was performed under the HPC Advisory Council HPC|works working group activities
  – Participating vendors: HP, Intel, Mellanox
  – Compute resource - HPC Advisory Council Cluster Center

• For more info please refer to
  – [www.intel.com](http://www.intel.com)
  – [www.mellanox.com](http://www.mellanox.com)
  – [http://cp2k.berlios.de](http://cp2k.berlios.de)
• CP2K is an atomistic and molecular simulations software for solid state, liquid, molecular and biological systems
• CP2k provides a general framework for different methods, such as:
  – Density functional theory (DFT) using a mixed Gaussian and plane waves approach (GPW)
  – Classical pair and many-body potentials
• CP2K is a freely available (GPL) program, written in Fortran 95
Objectives

- The presented research was done to provide best practices
  - MPI libraries comparisons
  - Interconnect performance benchmarking
  - CP2K Application profiling
  - Understanding CP2K communication patterns
  - CP2K performance optimization

- The presented results will demonstrate
  - Balanced compute environment determines application performance
  - Tips to tune MPI to achieve maximum CP2K scalability
Test Cluster Configuration

- **HP ProLiant SL2x170z G6 16-node cluster**
  - Six-Core Intel X5670 @ 2.93 GHz CPUs
  - Memory: 24GB per node
  - OS: CentOS5U5, OFED 1.5.3 InfiniBand SW stack

- **Mellanox ConnectX-2 InfiniBand QDR adapters and switches**

- **Fulcrum based 10Gb/s Ethernet switch**

- **MPI: Intel MPI 4, Open MPI 1.5.3 with KNEM 0.9.6, Platform MPI 8.0.1**

- **Compilers: Intel Compilers 11.1**

- **Application: CP2K version 2.2.196**

- **Libraries: Intel MKL 10.1, BLACS, ScaLAPACK 1.8.0**

- **Benchmark workload**
  - H2O-128.inp
About HP ProLiant SL6000 Scalable System

• Solution-optimized for extreme scale out

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

Mix and match configurations

Deploy with confidence

ProLiant SL170z G6
Large storage
-Web search and database apps

ProLiant SL160z G6
Large memory
-memory-cache apps

ProLiant z6000 chassis
Shared infrastructure
- fans, chassis, power

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

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

#1 Power Efficiency*
CP2K Benchmark Results – Open MPI

- **Input Dataset**
  - H2O-128.inp

- **MPI tuning enables nearly 18% performance gain at 16 nodes / 192 cores**
  - KNEM accelerates intra node communication
  - MPI RDMA optimization reduce inter-node communication latency
  - --mca btl_openib_eager_limit 65536 --mca btl_openib_max_eager_rdma 8 --mca btl_openib_eager_rdma_num 8

**CP2K**
(H2O-128.inp)

\[\text{Higher is better}\]

12-cores per node
CP2K Benchmark Results – Intel MPI

• Applying optimized parameters improves CP2K performance by 23%
  – Increase alignment for the sending buffer
  – Use right Alltoall and Alltoallv algorithm

Higher is better

12-cores per node
CP2K Benchmark Results – MPI Libraries

- Open MPI is better at smaller node count
- All tested MPI libraries have similar performance at 16 nodes

**CP2K**

(H2O-128.inp)

- Higher is better

12-cores per node
CP2K Benchmark Results – Interconnects

- Only InfiniBand enables CP2K application scalability
  - GigE can’t scale even on 2 nodes
  - 10GigE stops scaling after 2 nodes

CP2K
(H2O-128.inp)

Higher is better

12-cores per node
Both MPI collectives and point-to-point creates big communication time

- MPI_Alltoallv and MPI_Allreduce
- MPI_Waitall and MPI_Isend
Majority messages are smaller than 64KB
CP2K MPI Profiling – 10GigE vs IB

- 10GigE spends most time in communication rather than computation

![Bar chart showing CP2K (H2O-128.inp) comparison between User and MPI for 10GigE and InfiniBand QDR, with 48 Ranks.](chart.png)
• 10GigE has big communication overhead with MPI collectives
  – 22 times longer than InfiniBand QDR
CP2K Benchmark Summary

• **CP2K performance benchmark demonstrates**
  – InfiniBand QDR enables application performance and scalability
  – Neither GigE nor 10GigE meet CP2K network requirement

• **CP2K MPI profiling**
  – Large number of small messages are used by CP2K
  – MPI_Alltoallv, MPI_Alltoall, and MPI_Allreduce are major collectives
  – Point-to-point has big communication overhead
  – Interconnect latency is critical to CP2K performance

• **MPI tuning accelerates CP2K performance**
  – More than 20% at 16 nodes / 192 cores
Thank You
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