CP2K
Performance Benchmark and Profiling

April 2011
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

- [http://www.amd.com](http://www.amd.com)
- [http://www.dell.com/hpc](http://www.dell.com/hpc)
- [http://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 following was done to provide best practices
  - CP2K performance benchmarking
  - Interconnect performance comparisons
  - Understanding CP2K communication patterns
  - Ways to increase CP2K productivity
  - MPI libraries comparisons

- The presented results will demonstrate
  - The scalability of the compute environment
  - The capability of CP2K to achieve scalable productivity
  - Considerations for performance optimizations
Test Cluster Configuration

- Dell™ PowerEdge™ R815 11-node (528-core) cluster
- AMD™ Opteron™ 6174 (code name “Magny-Cours”) 12-cores @ 2.2 GHz CPUs
- 4 CPU sockets per server node
- Mellanox ConnectX-2 VPI adapters for 40Gb/s QDR InfiniBand and 10Gb/s Ethernet
- Mellanox MTS3600Q 36-Port 40Gb/s QDR InfiniBand switch
- Fulcrum based 10Gb/s Ethernet switch
- Memory: 128GB memory per node DDR3 1333MHz
- OS: RHEL 5.5, MLNX-OFED 1.5.2 InfiniBand SW stack
- MPI: Intel MPI 4, Open MPI 1.5.3 with KNEM 0.9.6, Platform MPI 8.0.1
- Compilers: Intel Compilers 11.1, PGI 11.4
- Application: CP2K version 2.2.196 (External libraries used: Intel MKL 10.1, FFTW3, BLACS, ScaLAPACK 1.8.0, LAPACK 3.3)
- Benchmark workload: H2O-256.inp
Dell™ PowerEdge™ R815 11-node cluster

- **HPC Advisory Council Test-bed System**

- **New 11-node 528 core cluster - featuring Dell PowerEdge™ R815 servers**
  - Replacement system for Dell PowerEdge SC1435 (192 cores) cluster system following 2 years of rigorous benchmarking and product EOL
    - System to be redirected to explore HPC in the Cloud applications

- **Workload profiling and benchmarking**
  - Characterization for HPC and compute intense environments
  - Optimization for scale, sizing and configuration and workload performance
  - Test-bed Benchmarks
    - RFPs
    - Customers/Prospects, etc
  - ISV & Industry standard application characterization
  - Best practices & usage analysis
Best of breed technologies and partners

Combination of AMD™ Opteron™ 6100 series platform and Mellanox ConnectX InfiniBand on Dell HPC

Solutions provide the ultimate platform for speed and scale
- Dell PowerEdge R815 system delivers 4 socket performance in dense 2U form factor
- Up to 48 core/32DIMMs per server – 1008 core in 42U enclosure

Integrated stacks designed to deliver the best price/performance/watt
- 2x more memory and processing power in half of the space
- Energy optimized low flow fans, improved power supplies and dual SD modules

Optimized for long-term capital and operating investment protection
- System expansion
- Component upgrades and feature releases
CP2K Performance – Interconnects

- **InfiniBand shows continuous gain as the cluster scales**
  - The only interconnect that enables higher scalability for CP2K
- **Ethernet performance does not scale beyond 1 node**
  - Both 10GigE and 1GigE performance plummets with 2 or more nodes
CP2K Performance – MPI Implementations

- **Platform MPI enables the highest scalability**
  - Up to 72% faster than Intel MPI on 8 nodes
  - Up to 19% faster than Open MPI with KNEM support on 8 nodes
- **Open MPI runs with KNEM support**
  - KNEM enables intra-node MPI communication for large messages

**CP2K Benchmark (H2O-256)**

- **Jobs/Hour**
- **Number of Nodes**
- **Higher is better**

48 Cores/Node
CP2K Performance – InfiniBand Multi-rail

- Dual-rail (Dual InfiniBand cards) enables better performance than single-rail
  - Up to 10% better at 11-node
- The benefit of dual-rail starts to show with 8 nodes
  - Expect to see more gain as the cluster size increases

![CP2K Benchmark](image)

- Higher is better
- Open MPI
- 48 Cores/Node
CP2K Performance – CPU Frequency

- Increasing CPU core frequency enables higher job efficiency
  - Up to 30% better job performance between 2200MHz vs 1400MHz
  - Up to 11% better job performance between 2200MHz vs 1800MHz

CP2K Benchmark
(H2O-256)

Jobs/ Hour

<table>
<thead>
<tr>
<th>Number of Nodes</th>
<th>1400MHz</th>
<th>1800MHz</th>
<th>2200MHz</th>
</tr>
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<tbody>
<tr>
<td>8</td>
<td>10</td>
<td>11</td>
<td>12</td>
</tr>
</tbody>
</table>

Higher is better

48 Cores/Node
CP2K Profiling – MPI/User Time Ratio

- **CP2K becomes communicative at a very fast pace**
  - Due to the high core counts per node
- **MPI communication time dominates the overall time**
  - Shows low latency interconnect such as InfiniBand is required for good scalability

![CP2K Profiling Graph](image)

**CP2K Profiling**

(H2O-256)

MPI/User Time Ratio

Number of Nodes

48 Cores/Node

Higher is better

<table>
<thead>
<tr>
<th>Number of Nodes</th>
<th>Percentage of Messages</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>MPI time: 40.00%</td>
</tr>
<tr>
<td></td>
<td>User time: 20.00%</td>
</tr>
<tr>
<td>2</td>
<td>MPI time: 40.00%</td>
</tr>
<tr>
<td></td>
<td>User time: 20.00%</td>
</tr>
<tr>
<td>4</td>
<td>MPI time: 30.00%</td>
</tr>
<tr>
<td></td>
<td>User time: 10.00%</td>
</tr>
<tr>
<td>8</td>
<td>MPI time: 60.00%</td>
</tr>
<tr>
<td></td>
<td>User time: 10.00%</td>
</tr>
<tr>
<td>11</td>
<td>MPI time: 70.00%</td>
</tr>
<tr>
<td></td>
<td>User time: 10.00%</td>
</tr>
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</table>
CP2K Profiling - Number of MPI Calls

- CP2K with this dataset uses an extensive list of MPI calls
  - 26 different MPI APIs are used
- The most used MPI function is MPI_Isend and Irecv
  - Each accounted for 42% of all MPI calls on a 11-node job
- MPI_Waitall represents a smaller ratio as size increases
  - From 26% down to 14% from 1 node to 11 node
The largest time consumer is calls MPI_Waitall
- MPI_Waitall uses for waiting communications to complete
- Occupies 44% of all MPI time for 1 node
- Occupies 24% of all MPI time for 11 node

Next on the list are MPI_Isend and MPI_Alltoallv
- MPI_Isend takes up 14% and MPI_Alltoallv takes 11% on a 11-node run
CP2K Profiling – MPI Message Sizes

- **Majority of the MPI message sizes are small message sizes**
  - In the range of 0B and 64B for 8 nodes or less
- **Messages increase accelerates with the node count increases**
  - Especially in the range of 65B and 256B for 11 nodes
- **Benefit of Multi-rail begins to emerge starting with 8-node**
  - As the number of smaller messages start to increase dramatically
CP2K Profiling – Aggregated Data Transfer

- **Aggregated data transfer refers to:**
  - Total amount of data being transferred in the network between all MPI ranks collectively

- **The total data transfer increases as the cluster scales**
  - As the cluster size reaches a new level, amount of data being driven would be doubled

- **Demonstrates the advantage and importance of scalable network interconnect**
  - InfiniBand QDR can deliver bandwidth needed to push 21TB of data across the network

[Bar chart showing aggregated data transfer for CP2K Profiling (H2O-256) across different numbers of nodes.]

**InfiniBand QDR**
CP2K Profiling – Data Transfer Per Process

- Data transferred to each MPI rank is driven down in “levels”
  - From 120GB (1 node) to 60GB (2, 4 nodes) to 30GB (8 nodes)
  - Aggregated Data Transferred doubled for 11 node, hence the increase in data per rank

- As the cluster scales, data is spread across to more processes
Summary

- **CP2K and this dataset shows a high demand for:**
  - Both CPU and network bandwidth throughput

- **Networking:**
  - InfiniBand shows as the preferred interconnect solution for any cluster size
  - Shows benefit for using dual-rail InfiniBand from 8-nodes and up
  - 10GigE and 1GigE do not scale for this application and dataset

- **CPU:**
  - The CPU frequency has a direct impact on job productivity

- **MPI:**
  - Platform MPI allows good scalability for CP2K among the other MPI tested

- **Data being transferred on the network**
  - Tends to increase in “levels” that can create heavy burden to network as cluster scales
Thank You
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