HPC ADVISORY COUNCIL

CP2K
Performance Benchmark and Profiling

April 2011

AMD The future is fusion

DELL

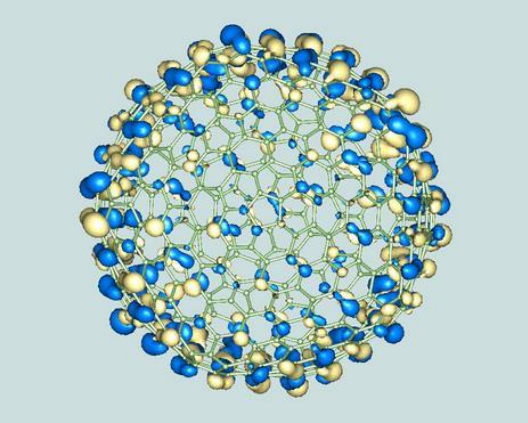
Mellanox TECHNOLOGIES

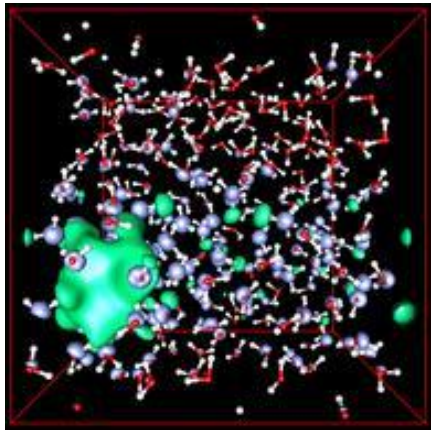
Note

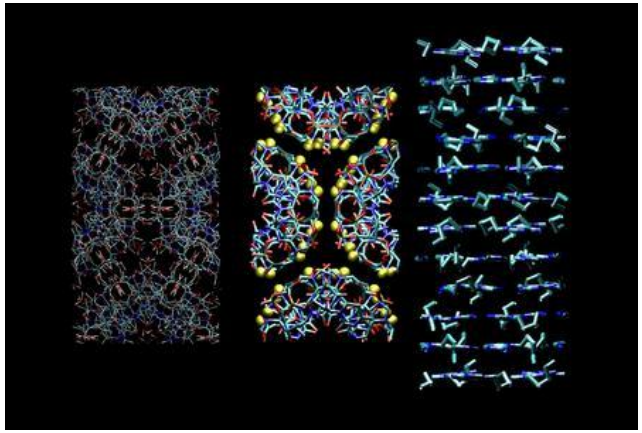
- **The following research was performed under the HPC Advisory Council activities**
  - Participating vendors: AMD, Dell, Mellanox
  - Compute resource - HPC Advisory Council Cluster Center
- **For more info please refer to**
  - http:// www.amd.com
  - http:// www.dell.com/hpc
  - http://www.mellanox.com
  - http://cp2k.berlios.de

CP2K

- **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

About Dell PowerEdge™ Platform Advantages

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

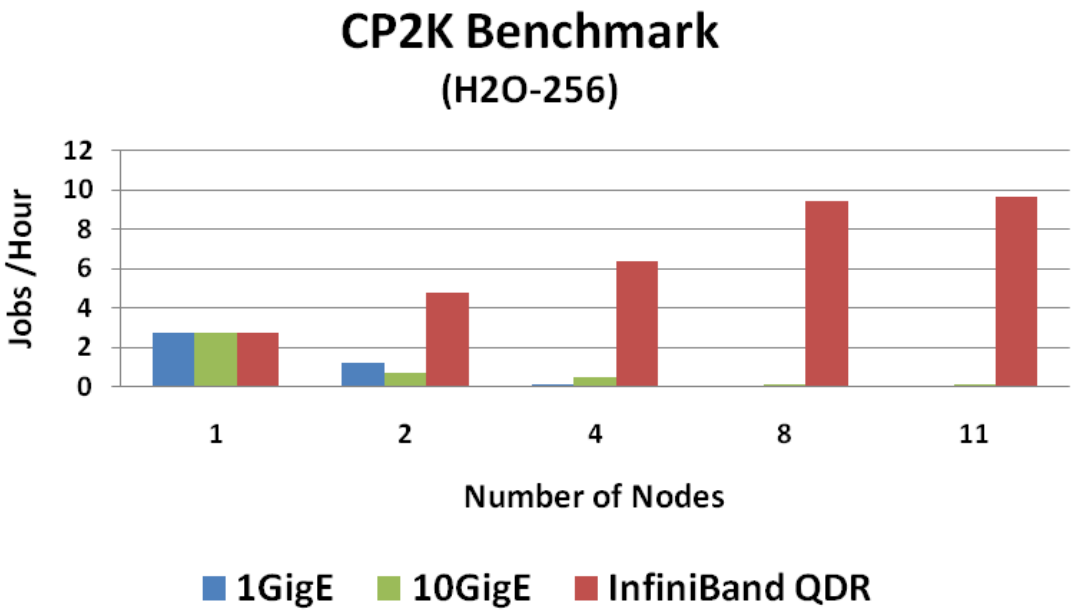
- 2x more memory and processing power in half of the space
- Energy optimized low flow fans, improved power supplies and dual SD modules

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

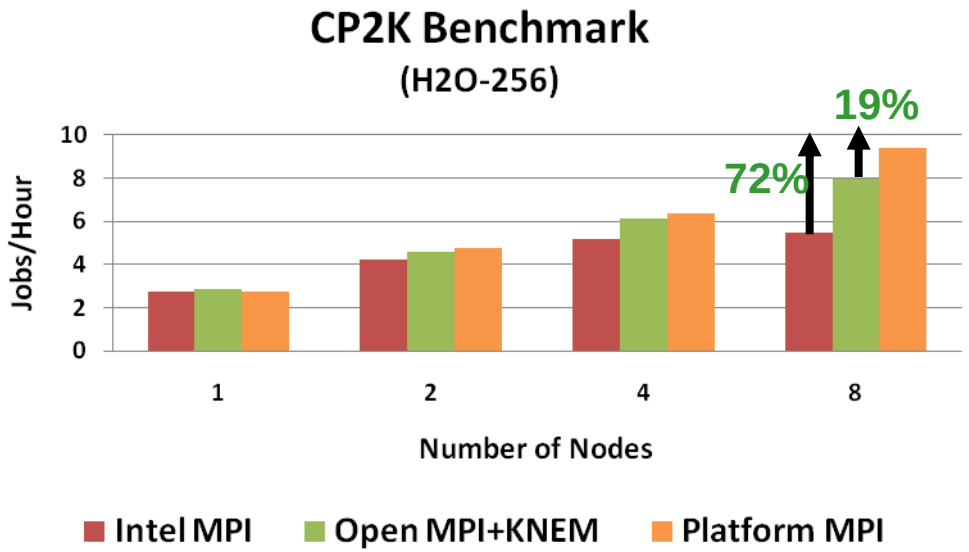


Higher is better

48 Cores/Node

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

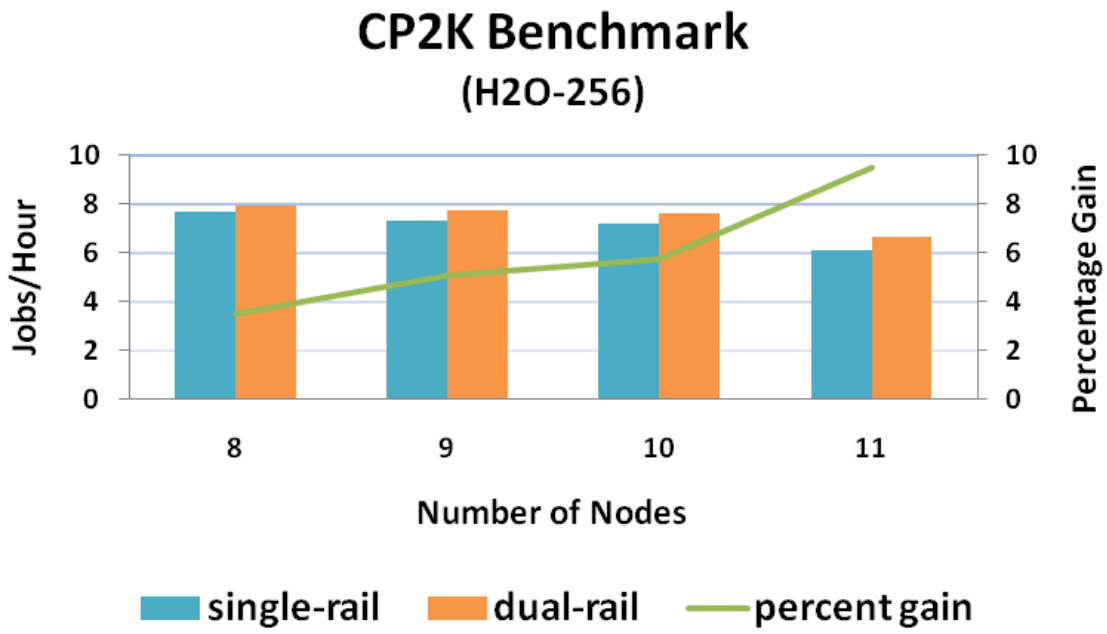


Higher is better

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



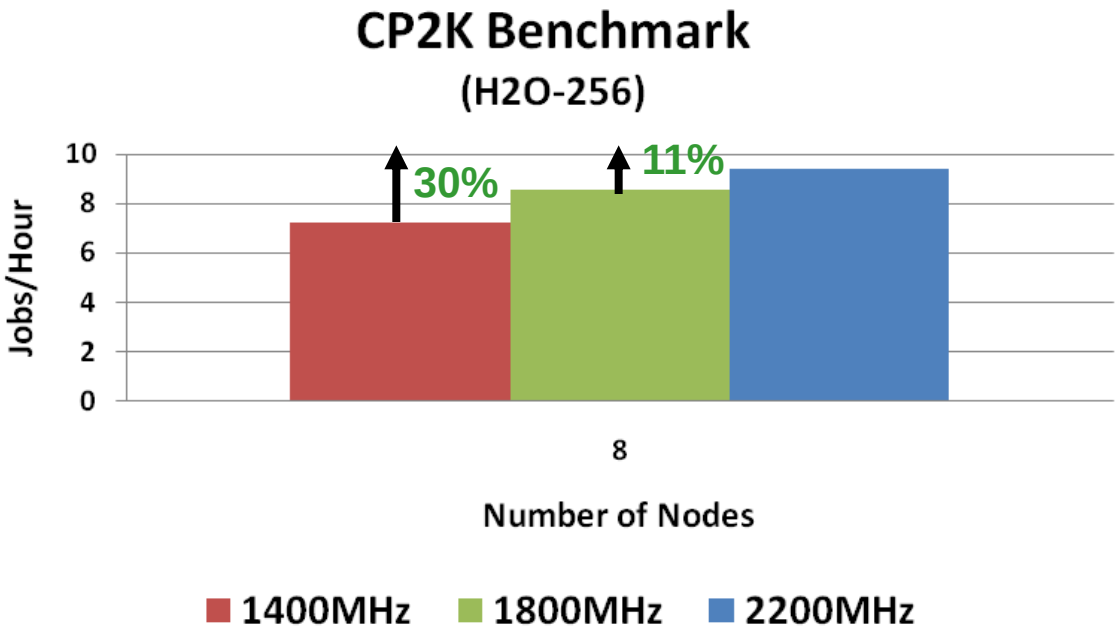
Higher is better

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

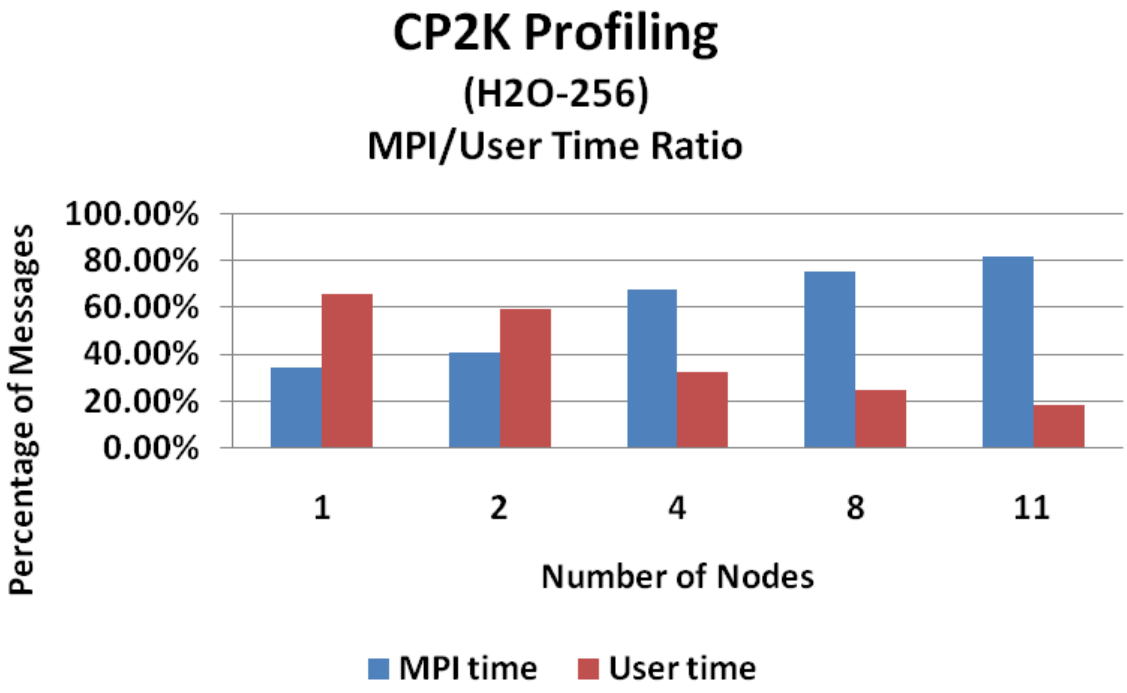


Higher is better

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

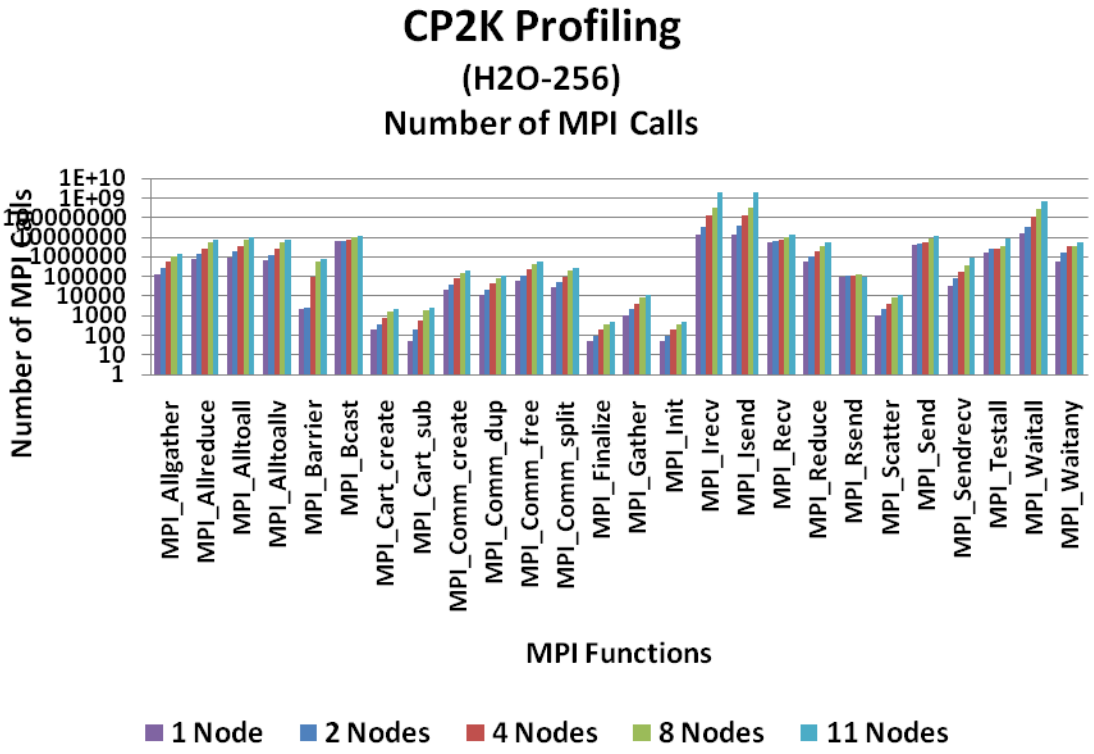


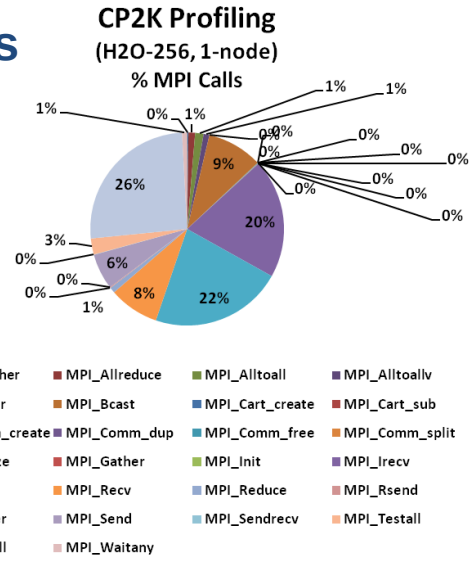
Higher is better

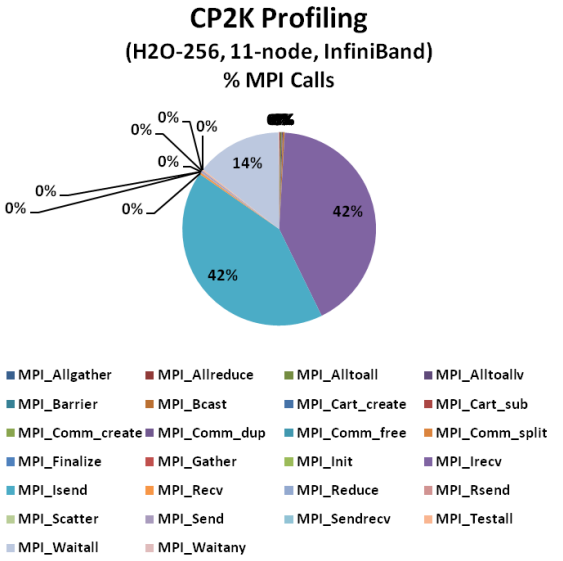
48 Cores/Node

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

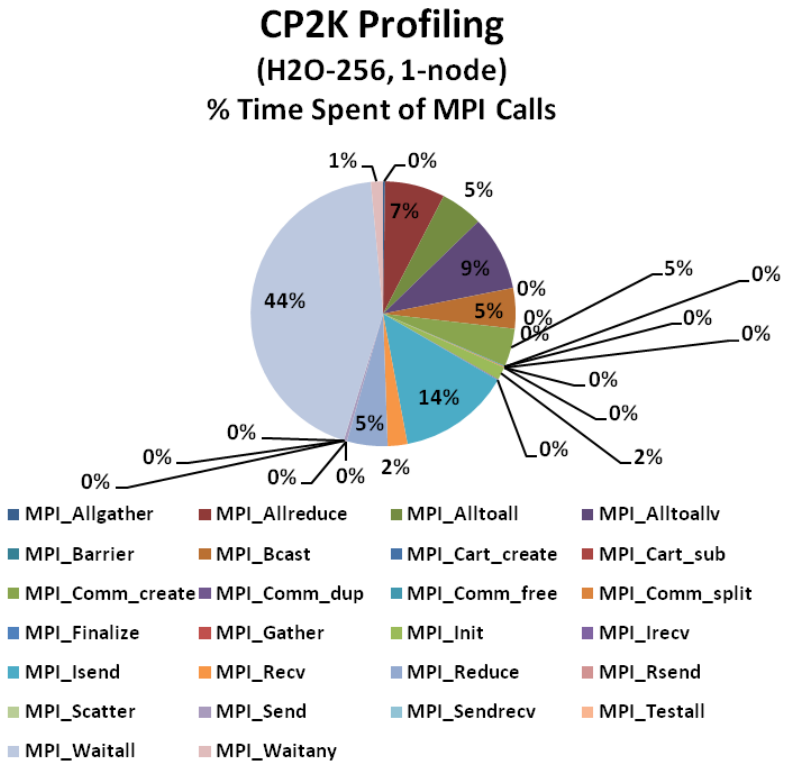


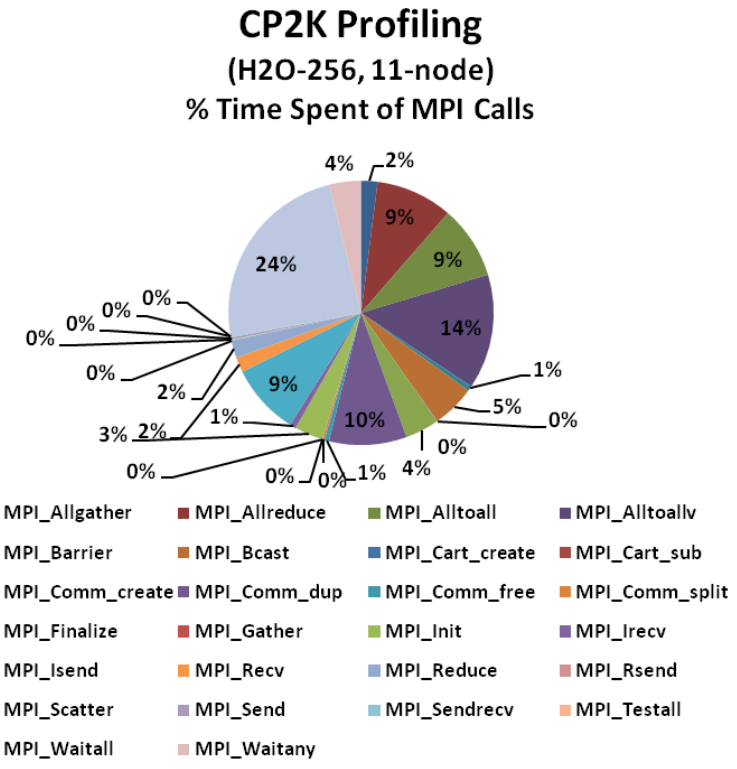




CP2K Profiling – Time Spent of MPI Calls

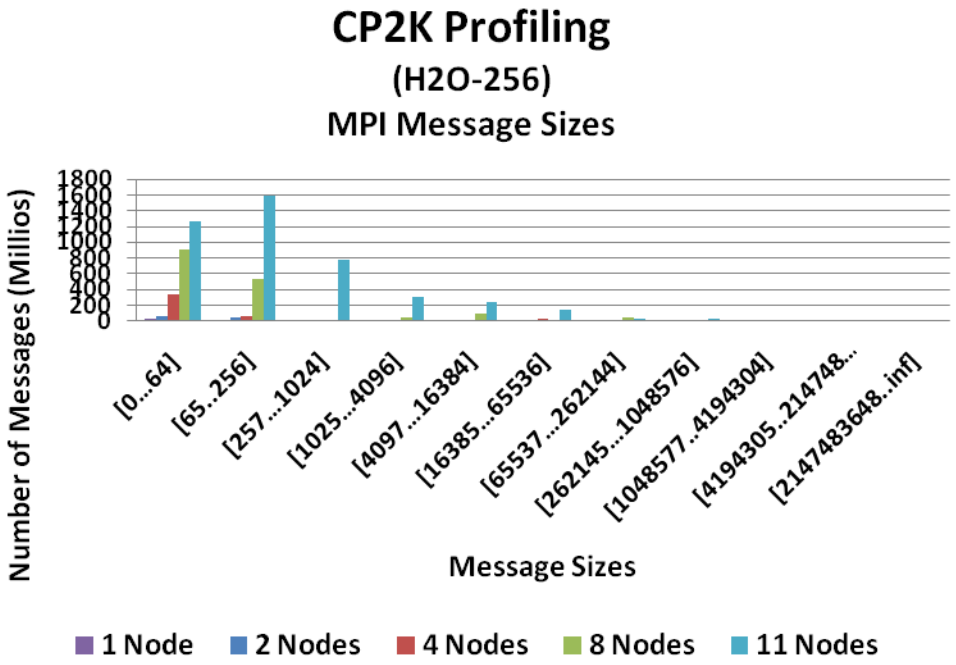
- **The largest time consumer is calls MPI_Waitall**
  - MPI_Waitall uses for waiting communications to complete
  - Occupies 44% of all MPI time for 1 node
  - Occupies 24% of all MPI time for 11 node
- **Next on the list are MPI_Isend and MPI_Alltoallv**
  - MPI_Isend takes up 14% and MPI_Alltoallv takes 11% on a 11-node run





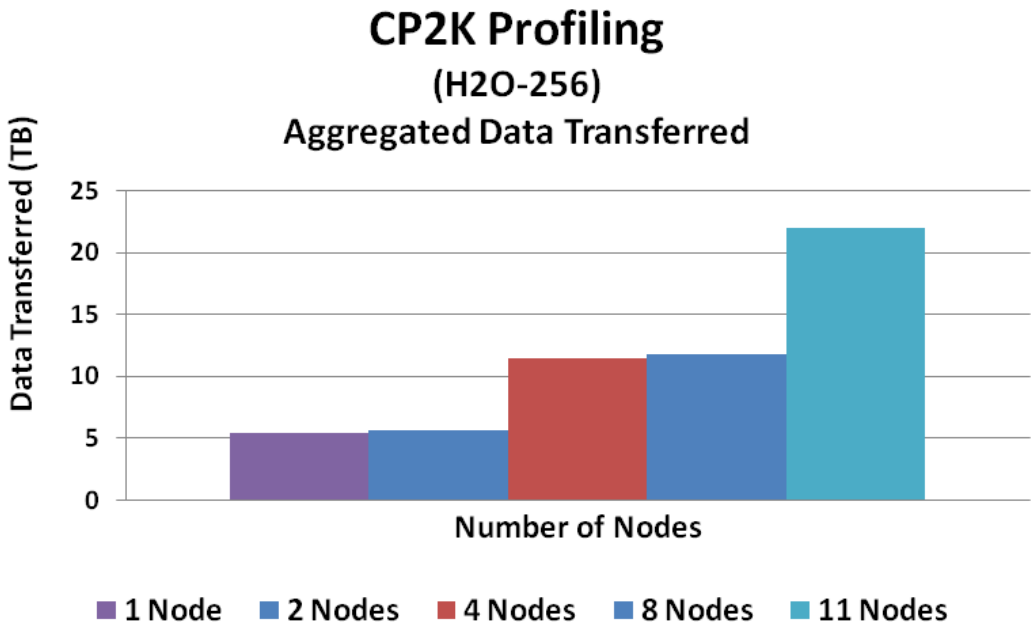
CP2K Profiling – MPI Message Sizes

- **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

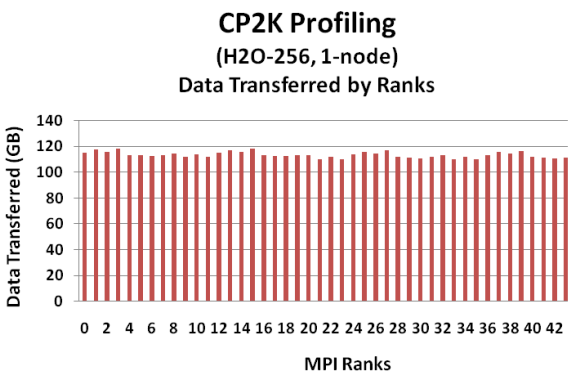
- **Aggregated data transfer refers to:**
  - Total amount of data being transferred in the network between all MPI ranks collectively
- **The total data transfer increases as the cluster scales**
  - As the cluster size reaches a new level, amount of data being driven would be doubled
- **Demonstrates the advantage and importance of scalable network interconnect**
  - InfiniBand QDR can deliver bandwidth needed to push 21TB of data across the network

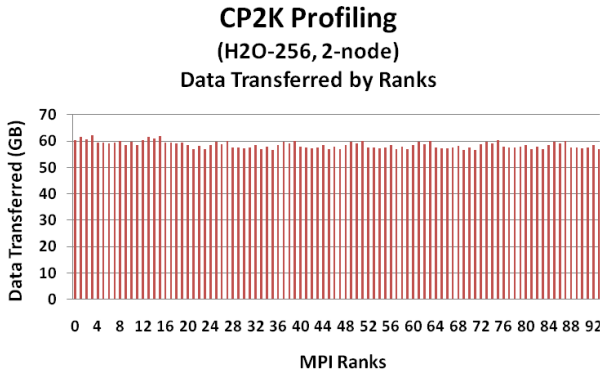


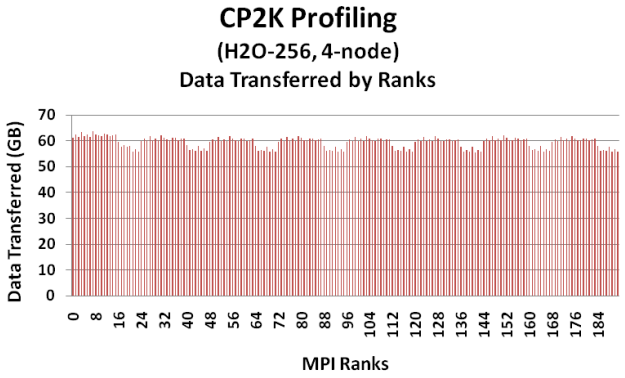
InfiniBand QDR

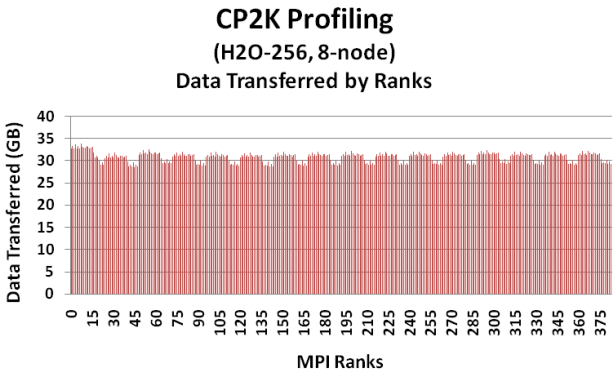
CP2K Profiling – Data Transfer Per Process

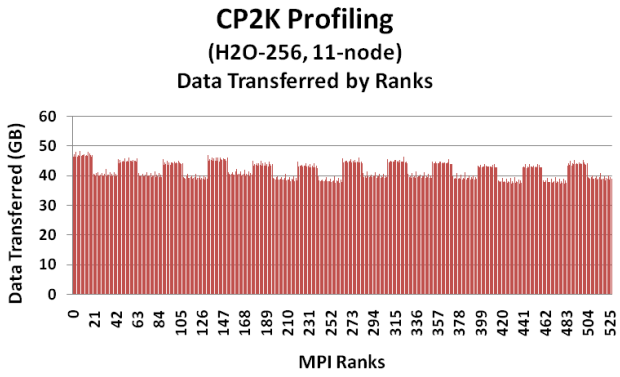
- **Data transferred to each MPI rank is driven down in "levels"**
  - From 120GB (1 node) to 60GB (2 ,4 nodes) to 30GB (8 nodes)
  - Aggregated Data Transferred doubled for 11 node, hence the increase in data per rank
- **As the cluster scales, data is spread across to more processes**











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

HPC Advisory Council