HPC ADVISORY COUNCIL

CP2K
Performance Benchmark and Profiling

April 2011

hp

Mellanox TECHNOLOGIES

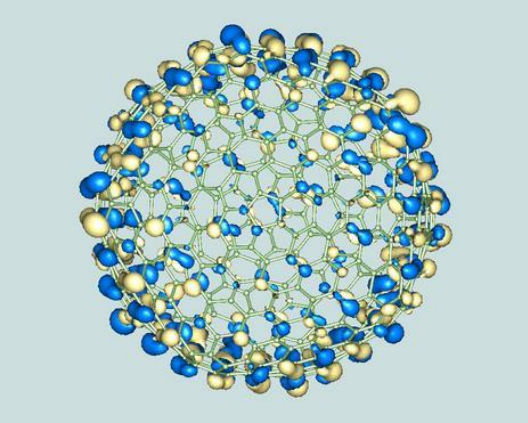
Note

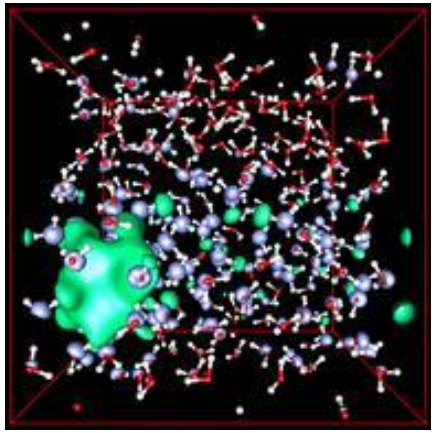
- **The following research was performed under the HPC Advisory Council HPC|works working group activities**
  - Participating vendors: HP, Intel, Mellanox
  - Compute resource - HPC Advisory Council Cluster Center

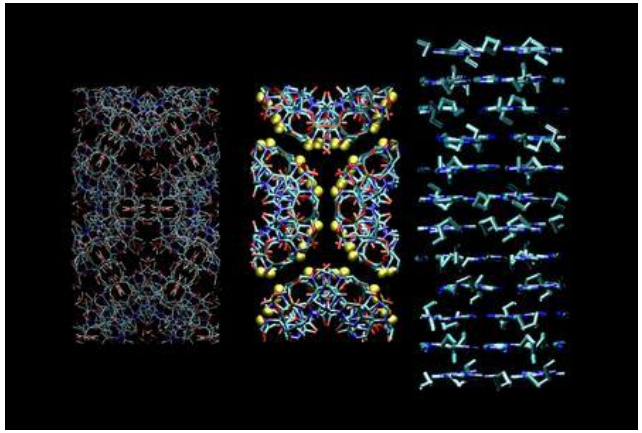
- **For more info please refer to**
  - http://www.hp.com/go/hpc
  - www.intel.com
  - www.mellanox.com
  - http://cp2k.berlios.de

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

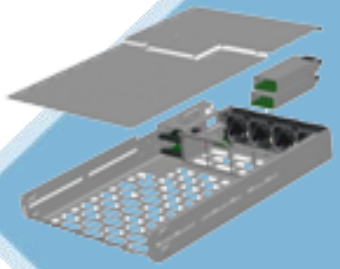
- **The presented results will demonstrate**
  - Balanced compute environment determines application performance
  - Tips to tune MPI to achieve maximum CP2K scalability

Test Cluster Configuration

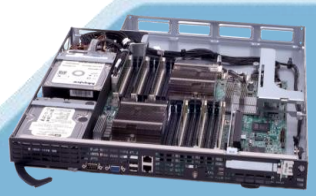
- **HP ProLiant SL2x170z G6 16-node cluster**
  - Six-Core Intel X5670 @ 2.93 GHz CPUs
  - Memory: 24GB per node
  - OS: CentOS5U5, OFED 1.5.3 InfiniBand SW stack
- **Mellanox ConnectX-2 InfiniBand QDR adapters and switches**
- **Fulcrum based 10Gb/s Ethernet switch**
- **MPI: Intel MPI 4, Open MPI 1.5.3 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

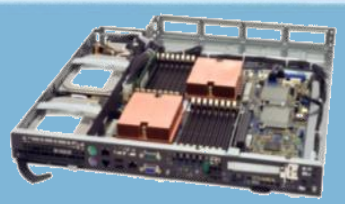
About HP ProLiant SL6000 Scalable System

- **Solution-optimized for extreme scale out**



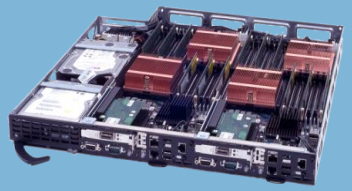
ProLiant z6000 chassis
Shared infrastructure
– fans, chassis, power





ProLiant SL160z G6 ProLiant SL165z G7
Large memory
-memory-cache apps

ProLiant SL170z G6
Large storage
-Web search and database apps



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

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

Mix and match configurations

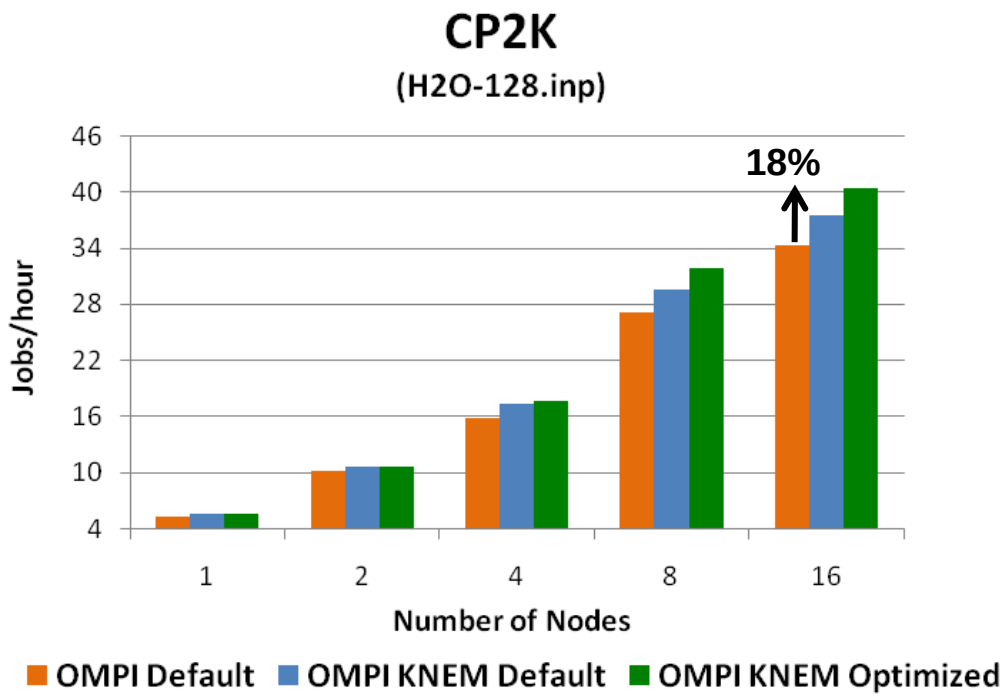
Deploy with confidence

#1 Power Efficiency*

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

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

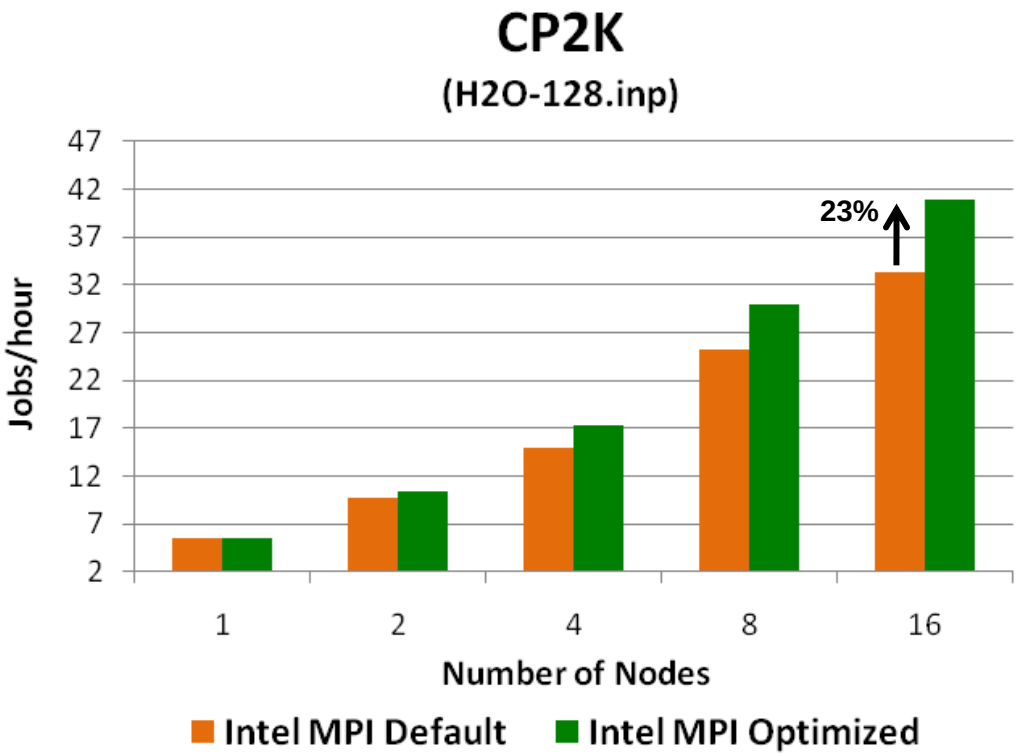


Higher is better

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
-

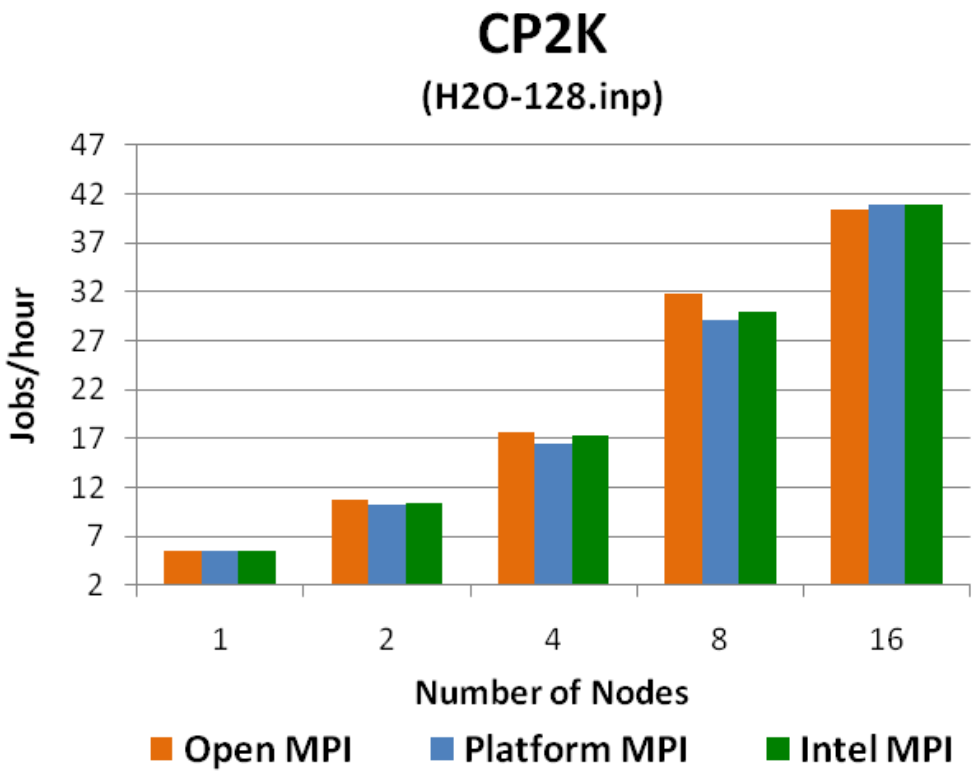


Higher is better

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

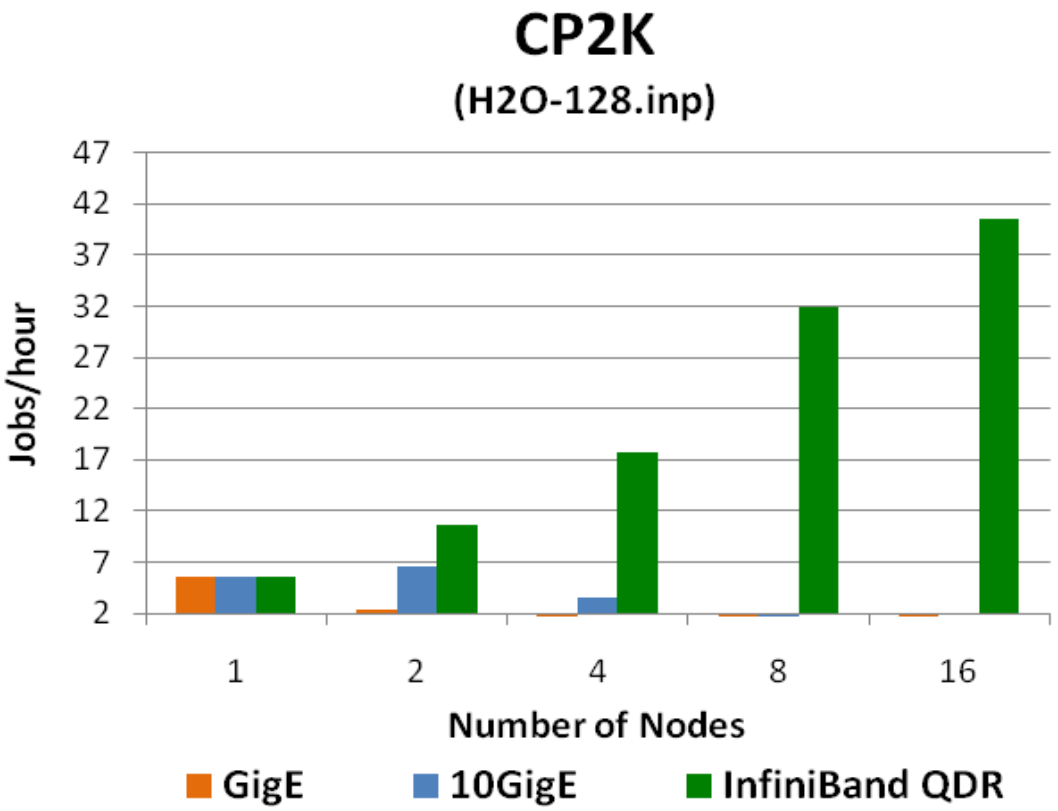


Higher is better

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

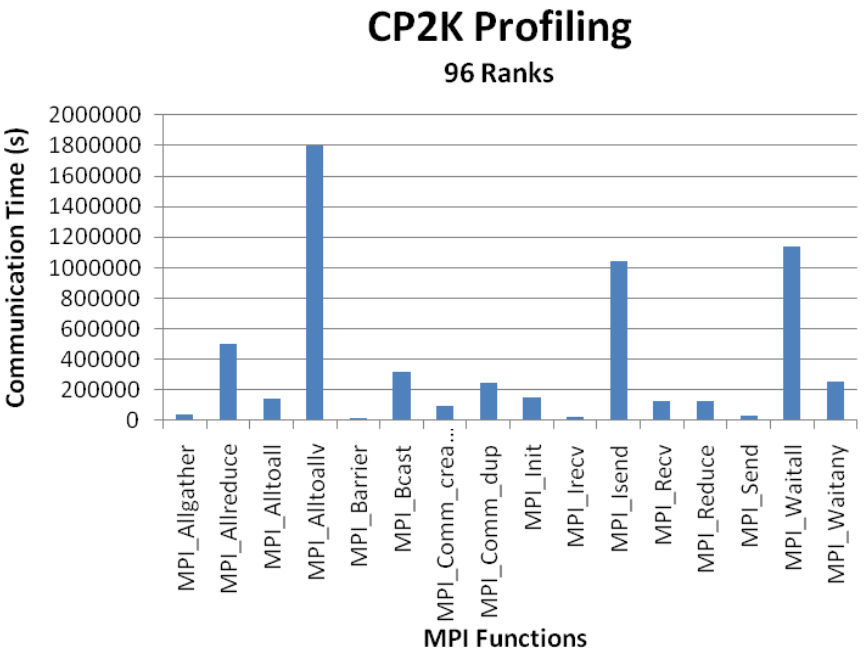


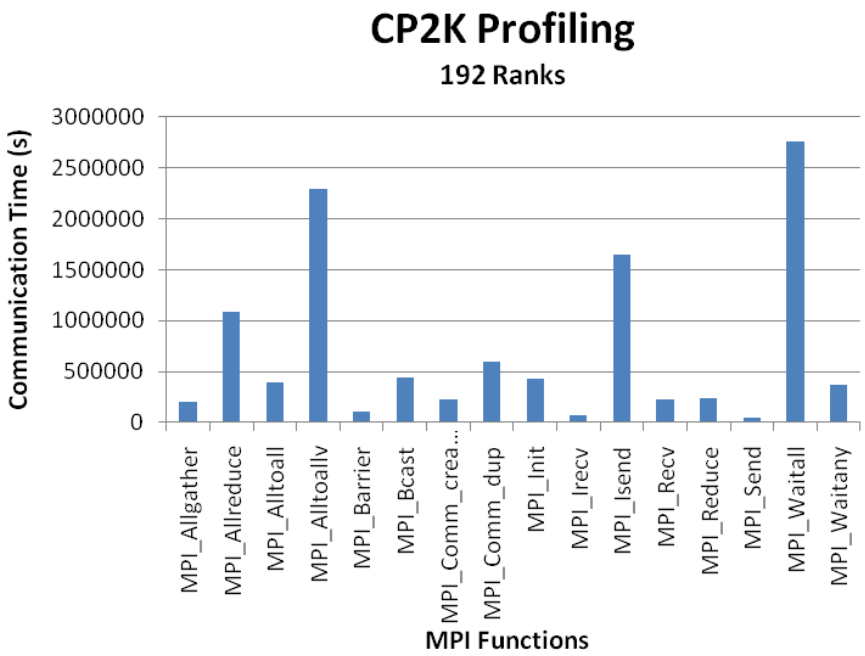
Higher is better

12-cores per node

CP2K MPI Profiling – MPI Functions

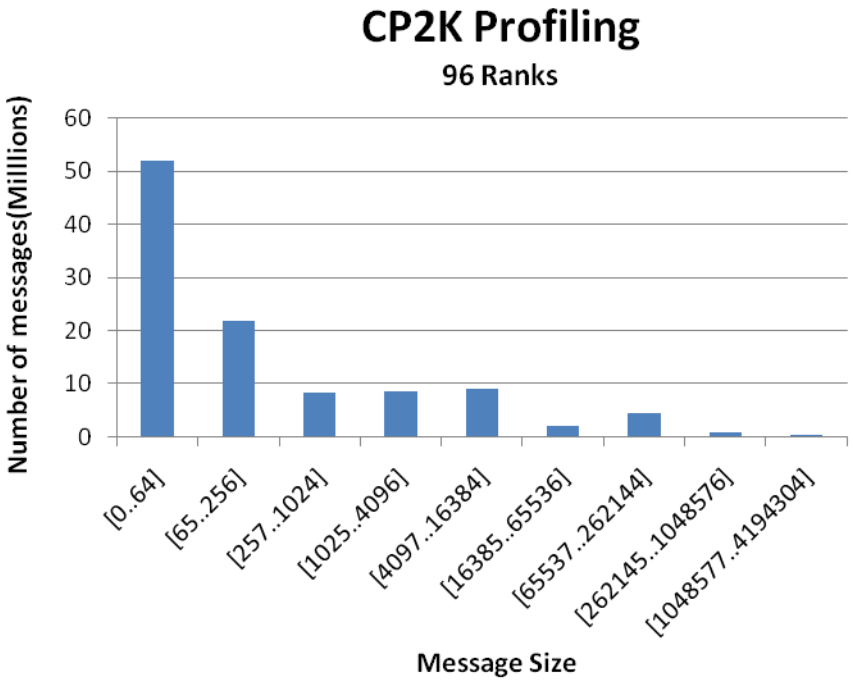
- **Both MPI collectives and point-to-point creates big communication time**
  - MPI_Alltoallv and MPI_Allreduce
  - MPI_Waitall and MPI_Isend

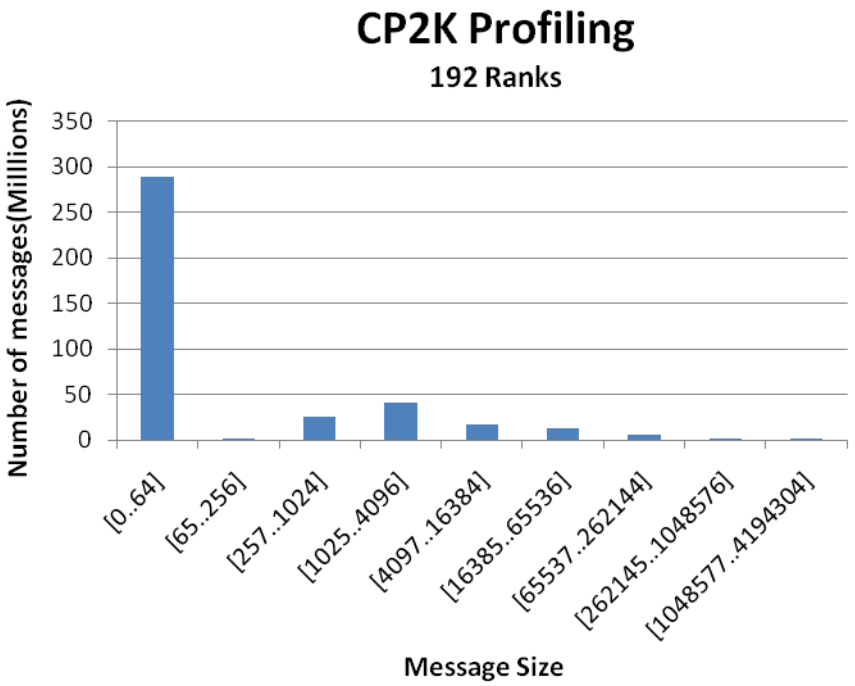




CP2K MPI Profiling – Message Size

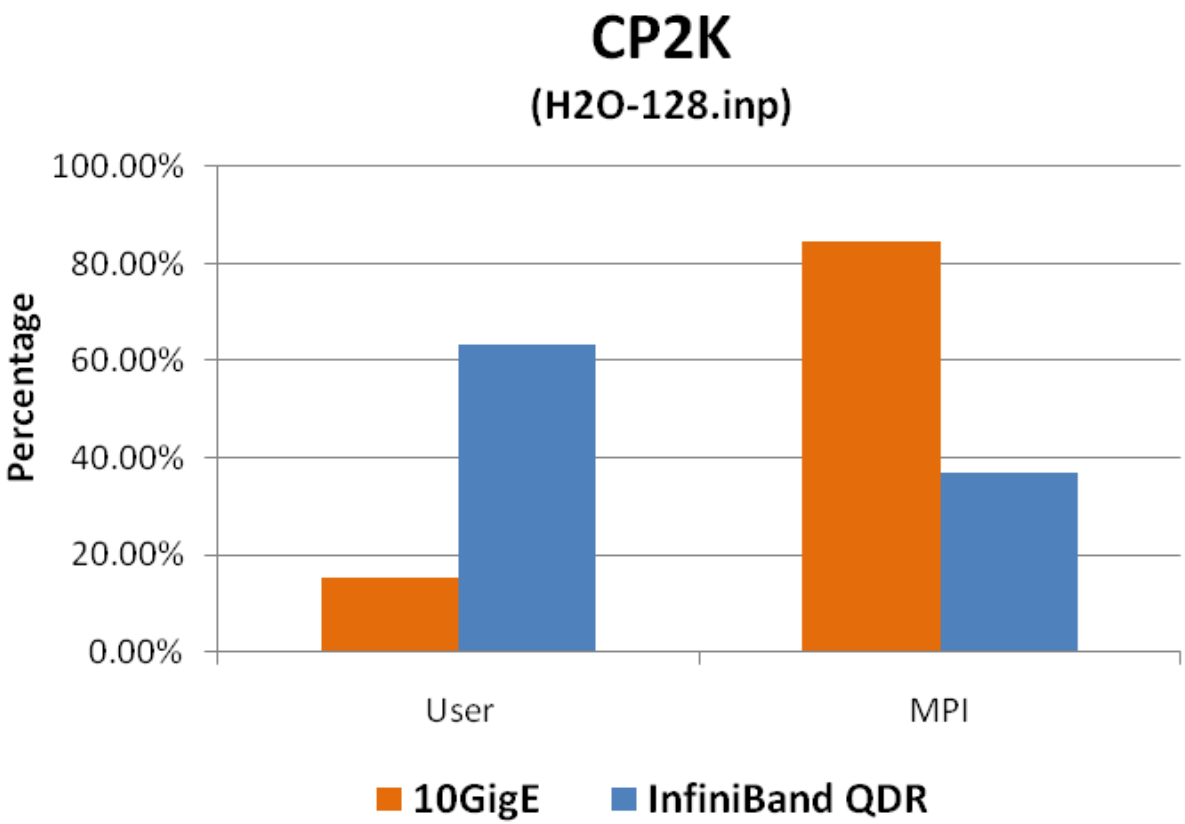
- **Majority messages are smaller than 64KB**





CP2K MPI Profiling – 10GigE vs IB

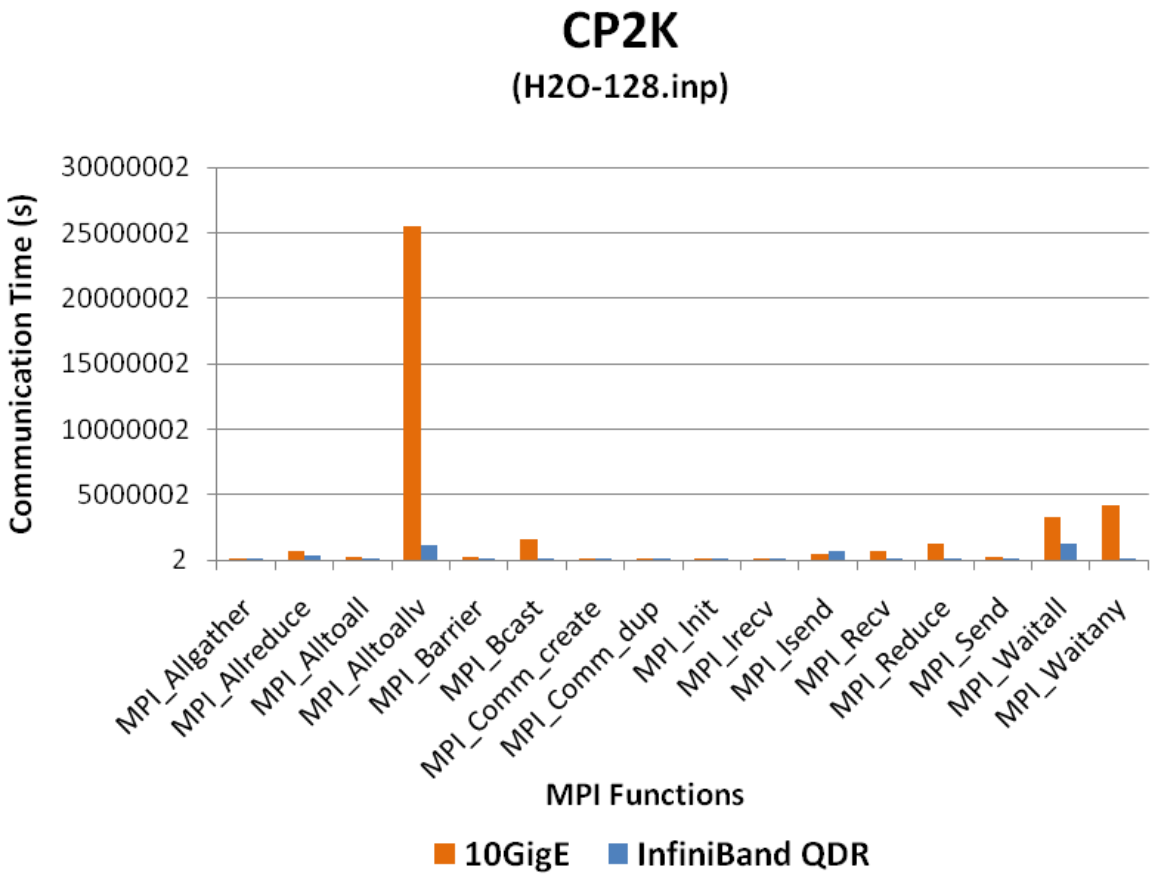
- **10GigE spends most time in communication rather than computation**



48 Ranks

CP2K MPI Profiling – 10GigE vs IB

- **10GigE has big communication overhead with MPI collectives**
  - 22 times longer than InfiniBand QDR



48 Ranks

CP2K Benchmark Summary

- **CP2K performance benchmark demonstrates**
  - InifiniBand 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

HPC Advisory Council