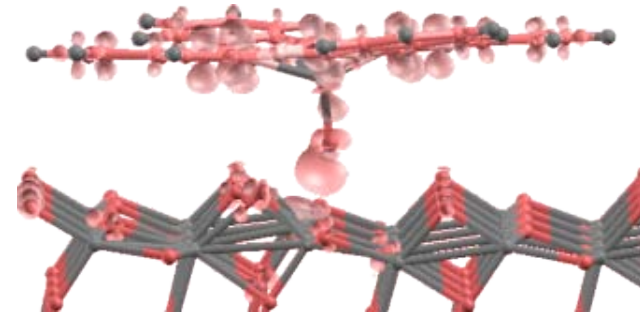# Quantum ESPRESSO Performance Benchmarking and Profiling

Sept 2010

Note

- **The following research was performed under the HPC Advisory Council activities**

  – Participating vendors: HP, Mellanox

  – Compute resource - HPC Advisory Council Cluster Center

- **For more info please refer to**

  – www.mellanox.com

  – http://www.hp.com/go/hpc

  – http://www.quantum-espresso.org

Quantum ESPRESSO

- Quantum ESPRESSO stands for opEn Source Package for Research in Electronic Structure, Simulation, and Optimization

- It is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale

- It is based on

  - Density-functional theory

  - Plane waves

  - Pseudopotentials (both norm-conserving and ultrasoft)

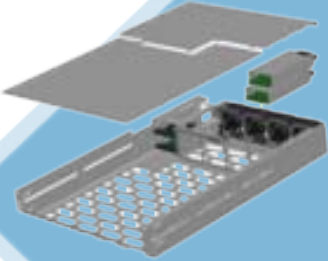- Open source under the terms of the GNU General Public License

Objectives

- **The presented research was done to provide best practices**

  – Quantum ESPRESSO performance benchmarking

    - Interconnect performance comparisons

  – Ways to increase ESPRESSO productivity

  – Power-efficient simulations

- **The presented results will demonstrate**

  – The scalability of the compute environment

  – Considerations for power saving through balanced system configuration
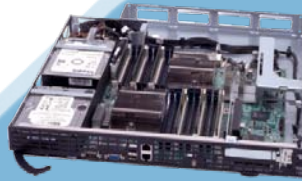
Test Cluster Configuration

- **HP ProLiant SL2x170z G6 16-node cluster**

  – Six-Core Intel X5670 @ 2.93 GHz CPUs

  – Memory: 24GB per node

  – OS: CentOS5U4, OFED 1.5.1 InfiniBand SW stack

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

- **Fulcrum based 10GigE switch**

- **MPI: Open MPI 1.4.1**

- **Application: Quantum ESPRESSO 4.1.2**

- **Benchmark Workload**

  – Medium size DEISA benchmark AUSURF112

    - Gold surface (112 atoms)

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

ProLiant SL160z G6   ProLiant SL165z G7

Large memory
-memory-cache apps
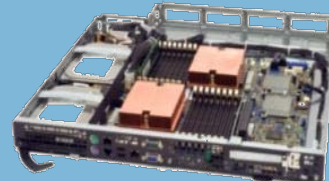
ProLiant SL170z G6

Large storage
-Web search and database apps

ProLiant z6000 chassis

Shared infrastructure
– fans, chassis, power
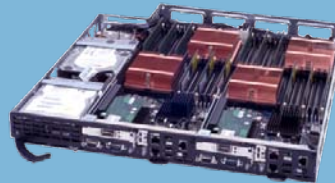
ProLiant SL2x170z G6

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

Quantum ESPRESSO Performance - Interconnect

- **Input Dataset**
  - DEISA benchmark AUSURF112
- **InfiniBand QDR enables higher scalability**
  - 360% higher performance than GigE at 8 nodes
  - 182% higher performance than 10GigE at 8 nodes
  - GigE stops scaling after 2 nodes
- **InfiniBand reduces electrical energy/job**
  - by 80% or more compared to GigE and 65% compared to 10GigE

Quantum ESPRESSO Benchmark
(AUSURF112)
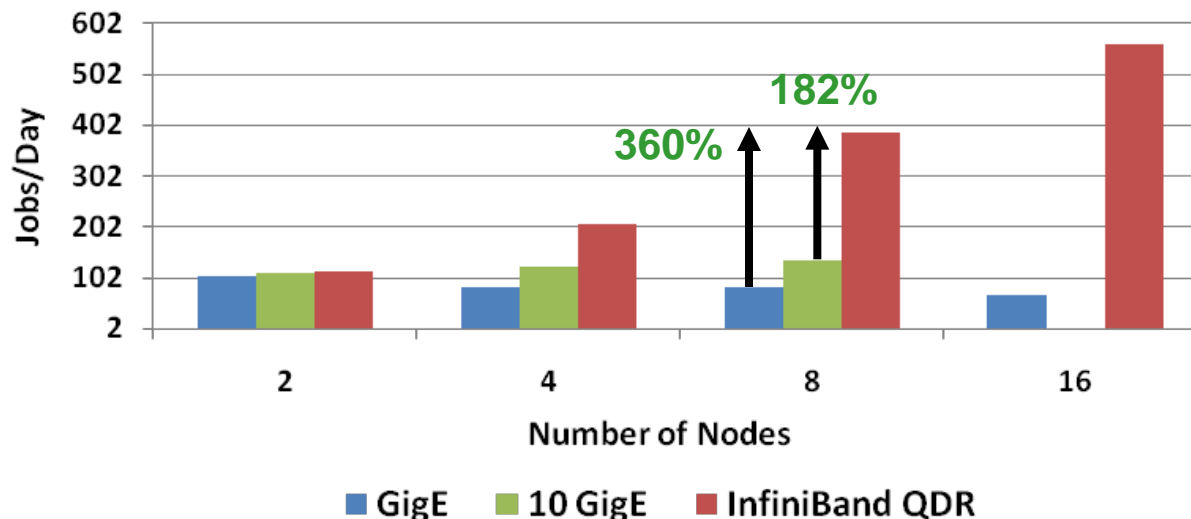
Higher is better

12 Cores/Node

# Quantum ESPRESSO Performance - Productivity

- **Input Dataset**
  - DEISA benchmark AUSURF112

- **Performance comparison**
  - 1 job mode: All cores per node used by single job
  - 2 jobs mode: Each job runs over half number of cores per socket
  - Running 2 jobs in parallel delivers 53% higher productivity than single job alone
    - Performance advantage grows as cluster size increases

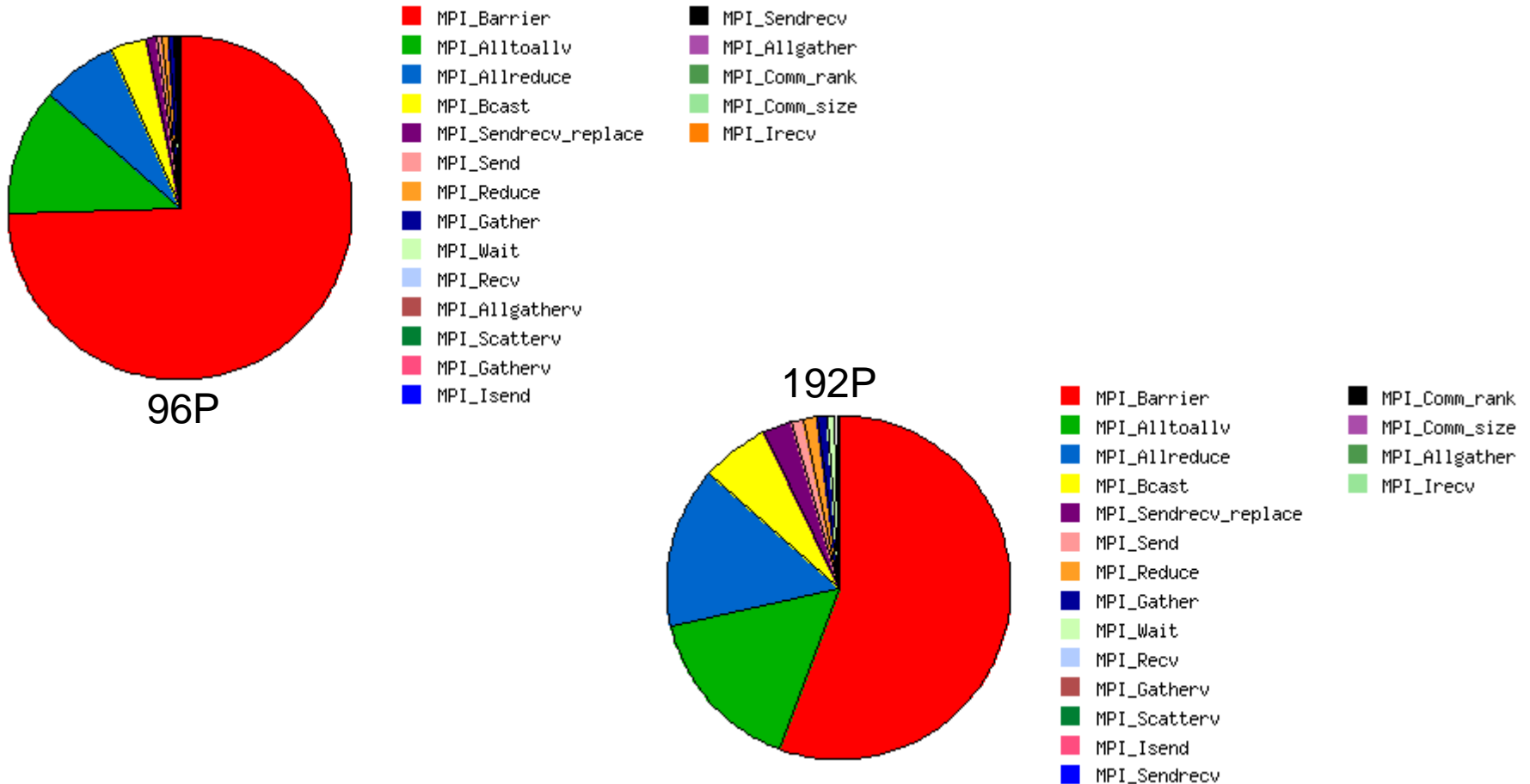## Quantum ESPRESSO Benchmark Results
(AUSURF112)
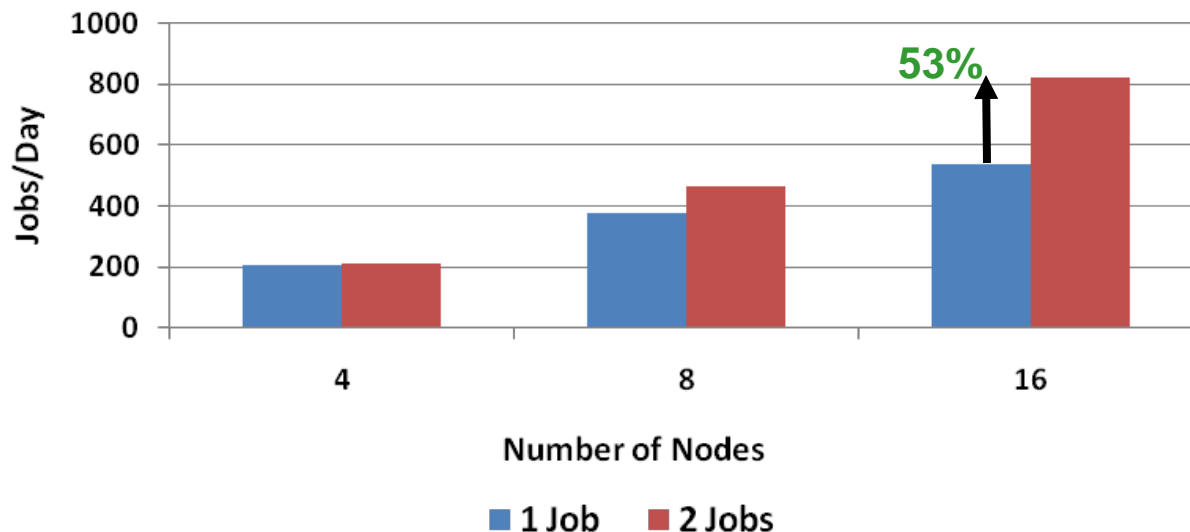
Higher is better

192 cores/16Nodes

- **MPI_Barrier, MPI_Alltoallv, and MPI_Addreduce generates most communication overhead**
- **MPI_Allreduce and MPI_Alltoallv overhead grow faster than other function**

Quantum ESPRESSO Benchmark Summary

- **Interconnect comparison shows**
  - InfiniBand delivers superior performance in every cluster size
  - Low latency InfiniBand enables much higher scalability than10GigE and GigE

- **Customized job placement increases application productivity**
  - 53% more jobs can be completed by running 2 jobs concurrently

- **InfiniBand QDR saves power**
  - Reduces power consumption/job by
    - 80% or more compared to GigE
    - 65% or more compared to 10GigE

- **MPI Profiling shows interconnect latency is the key to enable Quantum ESPRESSO scalability**

Thank You

HPC Advisory Council

NETWORK OF EXPERTISE