Quantum ESPRESSO Performance Benchmarking and Profiling

Sept 2010
• 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)
About HP ProLiant SL6000 Scalable System

• Solution-optimized for extreme scale out

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

- ProLiant SL165z G7

- 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

* 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

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### Quantum ESPRESSO Benchmark Results
(AUSURF112)

![Bar chart showing performance comparison between 1 job and 2 jobs mode.](chart)

- **Jobs/Day**
  - 0
  - 200
  - 400
  - 600
  - 800
  - 1000

- **Number of Nodes**
  - 4
  - 8
  - 16

- **Legend**
  - 1 Job
  - 2 Jobs

Higher is better

192 cores/16Nodes
Quantum ESPRESSO MPI Profiling – MPI Time

- 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 than 10GigE 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