CPMD Performance
With MPI Collectives Acceleration

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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

We would like to thank Mellanox for providing early access to its MPI Collectives Acceleration solution (FCA version 2.1)

For more info please refer to
- http://www.hp.com/go/hpc
- www.intel.com
- www.mellanox.com
- http://www.cpmd.org
Objectives

- The presented research was done to provide best practices
  - CPMD interconnect performance benchmarking
  - Application profiling
  - Understanding CPMD communication patterns

- Preview on available MPI collectives accelerations

- First performance results with CPMD
  - Utilizing MPI collectives accelerations
Car-Parrinello Molecular Dynamics (CPMD)

- CPMD
  - A parallelized implementation of density functional theory (DFT)
  - Particularly designed for ab-initio molecular dynamics
  - Brings together methods
    - Classical molecular dynamics
    - Solid state physics
    - Quantum chemistry
  - CPMD supports MPI and Mixed MPI/SMP
  - CPMD is distributed and developed by the CPMD consortium
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 1.5.2 InfiniBand SW stack

- Mellanox ConnectX-2 adapters and switches

- MPI: Open MPI 1.4.3

- Mellanox Fabric Collective Accelerator™ (FCA™) version 2.1

- Application: CPMD 3.13.2

- Benchmark Workload
  - C120 - 120 carbon atoms
About HP ProLiant SL6000 Scalable System

• Solution-optimized for extreme scale out

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

Mix and match configurations

Deploy with confidence

ProLiant SL160z G6
Large memory
-memory-cache apps

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

ProLiant z6000 chassis
Shared infrastructure
- fans, chassis, power

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

• Mellanox Fabric Collectives Accelerator (FCA)
  – Utilized hardware accelerations on the adapter (CORE-Direct)
  – Utilized managed switches capabilities (iCPU)
  – Accelerating MPI collectives operations
  – The world first complete solution for MPI collectives offloads

• FCA 2.1 supports accelerations/offloading for
  – MPI Barrier
  – MPI Broadcast
  – MPI AllReduce and Reduce
  – MPI AllGather and AllGatherV
Software Layers Overview

Running CPMD without FCA accelerations

Running CPMD with FCA accelerations

MPI

FCA

InfiniBand Driver

CORE-Direct API

InfiniBand HCA (with CORE Direct support)

Switch (with iCPU)
• **FCA accelerates CPMD performance up to 35%**
  - At 16 nodes, 192 cores
  - Performance benefit increases with cluster size – higher benefit expected at larger scale
Intel compiler enables higher performance with CPMD
- At 16 nodes, 192 cores

CPMD Benchmark (C120)

- Higher is better
• InfiniBand QDR enables higher application scalability
• MPI collectives generates most communication overhead
  – MPI_Alltoall, MPI_Barrier, MPI_Allreduce
  – MPI_Barrier overhead increases faster than rest function
CPMD – MPI Profiling

- FCA accelerates application by faster communication/computations
CPMD Benchmark Summary

- **MPI Collectives accelerations can dramatically accelerate HPC applications performance**
  - The data presented here reviewed acceleration at small scale
  - Large scale systems will get bigger benefit from such acceleration

- **CPMD MPI profiling**
  - Alltoall, Allreduce, and Barrier are the main MPI routine impacts CPMD performance

- **FCA package has proven to accelerate application even at small scale**
  - Both communication and computation time can be reduced
  - Nearly 34% at 16 nodes for CPMD
  - Higher performance boost expected at larger scale
Thank You
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