NAMD
GPU Performance Benchmark

March 2011
• The following research was performed under the HPC Advisory Council activities
  – Participating vendors: Dell, Intel, Mellanox
  – Compute resource - HPC Advisory Council Cluster Center

• For more info please refer to
  – http://www.dell.com
  – http://www.intel.com
  – http://www.mellanox.com
  – http://www.ks.uiuc.edu/Research/namd/
NAMD

- A parallel molecular dynamics code that received the 2002 Gordon Bell Award
- Designed for high-performance simulation of large biomolecular systems
  - Scales to hundreds of processors and millions of atoms
- Developed by the joint collaboration of the Theoretical and Computational Biophysics Group (TCB) and the Parallel Programming Laboratory (PPL) at the University of Illinois at Urbana-Champaign
- NAMD is distributed free of charge with source code
Objectives

- The presented research was done to provide best practices
  - NAMD performance benchmarking
  - Interconnect performance comparisons
  - Ways to increase NAMD productivity
  - Power-efficient simulations

- The presented results will demonstrate
  - The scalability of the compute environment
  - Considerations for performance optimization
Test Cluster Configuration

• **Dell™ PowerEdge™ C6100 4-node cluster**
  - Six-Core Intel X5670 @ 2.93 GHz CPUs, 24GB memory per node
  - OS: RHEL5 Update 5, OFED 1.5.2 InfiniBand SW stack

• **Dell™ PowerEdge™ C410x PCIe Expansion Chassis**
  - 4 NVIDIA® Tesla C2050 “Fermi” GPUs

• **Mellanox ConnectX-2 VPI Mezzanine cards for InfiniBand &10Gb Ethernet**

• **Mellanox MTS3600Q 36-Port 40Gb/s QDR InfiniBand switch**

• **Fulcrum based 10Gb/s Ethernet switch**

• **CUDA driver and runtime version 3.2**

• **Application: NAMD 2.7 (Linux-x86_64 -CUDA and ibverbs-CUDA distros)**

• **Benchmark Workloads:**
  - STMV (virus) benchmark (1,066,628 atoms, periodic, PME)
  - F1ATPase benchmark (327,506 atoms, periodic, PME)
NAMD Performance – GPUs

- Dataset: STMV (virus) benchmark (1,066,628 atoms, periodic, PME)
- Up to 138% higher performance with 4 GPUs vs 1 GPU on a single node
- Up to 60% higher performance 4-node each with single GPU versus 4 GPUs on a single node

![NAMD Benchmark](image)

Higher is better

InfiniBand QDR
12 Cores/Node
NAMD Performance – Interconnect

- **InfiniBand provides the highest performance as the cluster scales**
  - Up to 210% higher performance than 1GigE at 4-node
  - Up to 20% higher performance than 10GigE at 4-node

- **1GigE provides no job gain after 2 nodes**
  - GPU communications between nodes become a significantly burden to the network

![NAMD Benchmark](chart)
NAMD Performance – Scalability

- InfiniBand enables higher scalability – nearly 100%
- Only 31% of the system compute capability can be utilized with 1GigE

Higher is better

12 Cores/Node
NAMD Performance – GPU utilization

• **Dataset**
  - STMV (virus) benchmark (1,066,628 atoms, periodic, PME)

• **Using GPUs in computation shows benefit**
  - Results show that 92% gain in additional productivity with the use of 1 GPU per node
  - ibverbs+cuda – using GPU for computations, nodes connected via InfiniBand
  - ibverbs – no use of GPUs for the simulations, only CPUs, nodes connected via InfiniBand

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**NAMD Benchmark**

(stmv, 1GPU/node)

Higher is better

<table>
<thead>
<tr>
<th>Number of Nodes</th>
<th>ibverbs+cuda</th>
<th>ibverbs</th>
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</table>

92%

12 Cores/Node
NAMD Performance Result – GPU computation

- **Dataset**
  - F1ATPase benchmark (327,506 atoms, periodic, PME)

- **Utilizing GPUs in computation does not demonstrate benefit**
  - Results show that utilizing additional GPUs does not equal to performance improve
  - Due to the small size of the dataset
  - ibverbs+cuda – using GPU for computations, nodes connected via InfiniBand
  - ibverbs – no use of GPUs for the simulations, only CPUs, nodes connected via InfiniBand

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**NAMD Benchmark**
(f1atpase, 1GPU/node)

Higher is better

12 Cores/Node
Summary

• **Interconnects comparison for NAMD**
  
  – InfiniBand enables the highest performance and best GPU cluster scalability

• **Spreading GPUs to more nodes improves job productivity**
  
  – Distributing the GPUs across the cluster to allow the full GPU potential to unleash

• **NAMD can benefit performance boost with GPUs**
  
  – The STMV dataset shows big performance advantage with GPU
  
  – The F1ATPase dataset shows no performance gain due to its small size
Thank You
HPC Advisory Council