LAMMPS Performance Benchmark and Profiling

September 2010
• The following research was performed under the HPC Advisory Council activities

• For more info please refer to
  – http://www.dell.com
  – http://www.intel.com
  – http://www.mellanox.com
• **Large-scale Atomic/Molecular Massively Parallel Simulator**
  - Classical molecular dynamics code which can model:
    • Atomic
    • Polymeric
    • Biological
    • Metallic
    • Granular, and coarse-grained systems

• **LAMMPS runs efficiently in parallel using message-passing techniques**
  - Developed at Sandia National Laboratories
  - An open-source code, distributed under GNU Public License
Objectives

• The following was done to provide best practices
  – LAMMPS performance benchmarking
  – Interconnect performance comparisons
  – Understanding LAMMPS communication patterns
  – Power-efficient simulations

• The presented results will demonstrate
  – The scalability of the compute environment to provide nearly linear application scalability
  – The capability of LAMMPS to achieve scalable productivity
  – Considerations for power saving through balanced system configuration
Test Cluster Configuration

• **Dell™ PowerEdge™ M610 14-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 InfiniBand adapters and switches**

• **MPI:** Intel MPI 4, MVAPICH2 1.5, Open MPI 1.4.2, Platform MPI 7.1

• **Compilers** Intel Compilers 11.1, GNU 4.1.2

• **Libraries:** Intel MKL 10.2.4.032, fftw-2.1.5

• **Application:** LAMMPS-30Aug10

• **Benchmark Workload**
  - Rhodo - Rhodopsin protein in solvated lipid bilayer, CHARMM force field with a 10 Angstrom LJ cutoff
**LAMMPS Performance Result – Interconnect**

- **InfiniBand enables higher scalability**
  - Up to 193% higher performance than Ethernet at 14 nodes
  - Four InfiniBand connected servers deliver nearly the same performance vs 14 Ethernet connected servers

**LAMMPS Benchmark**
(Scaled-size Rhodopsin Protein)

- **Performance Rating** = 32,000 atoms x the number of cores divided by the wall-clock simulation time

**Higher is better**

**Number of Nodes**

1. GigE
2. InfiniBand QDR

**12 Cores/Node**
LAMMPS Performance Result - Scalability

- InfiniBand enables higher scalability – more than 85% at 14 nodes
- Less than 30% of the system compute capability can be utilized with Ethernet at 14 nodes

**LAMMPS Benchmark**
(Scaled-size Rhodopsin Protein)

<table>
<thead>
<tr>
<th>Number of Nodes</th>
<th>Scaling Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>GigE: 100</td>
</tr>
<tr>
<td>2</td>
<td>GigE: 80</td>
</tr>
<tr>
<td>4</td>
<td>GigE: 60</td>
</tr>
<tr>
<td>8</td>
<td>GigE: 40</td>
</tr>
<tr>
<td>14</td>
<td>InfiniBand QDR:80</td>
</tr>
</tbody>
</table>

*Higher is better*

12 Cores/Node
LAMMPS Performance Result – Compilers and Libraries (Single node)

- Intel Compilers and MKL libraries provides higher performance versus GNU compilers and FFTW libraries
  - ~41% higher per process basis
  - ~46% higher per node basis

Higher is better
Intel Compilers enables 25% higher performance than GNU Compilers and FFTW library.
Intel MPI and Platform MPI demonstrate better performance
- Used with Intel compilers and MKL libraries together to deliver the highest performance
- 9% gain compared to Open MPI at 14-node
• Running 2 jobs concurrently can provide slightly higher productivity
  – 2 jobs setup: 6 cores/node per job; 1 job setup: 12 cores/node
  – Up to 6% higher performance when 2 jobs running concurrently

LAMMPS Benchmark
(Scaled-size Rhodopsin Protein)
LAMMPS Profiling Result – # of MPI Calls

- MPI_Send, MPI_Allreduce and MPI_Waitany the mostly used calls

LAMMPS Profiling
(Scaled-size Rhodopsin Protein)

Number of Nodes

- 1 Node
- 2 Nodes
- 4 Nodes
- 8 Nodes
- 14 Nodes

Higher is better

12 Cores/Node
LAMMPS Profiling Result – % Time of MPI Calls

- Majority of communication time is spent on MPI_Send and MPI_Allreduce
  - Percentage time is relatively consistent as number of nodes increases
LAMMPS Profiling Result – # of Message/Sizes

- Majority of messages are small and medium messages
  - Messages around 64B and 64KB are mostly used
- Number of messages increases dramatically with the number of nodes

![LAMMPS Profiling Graph](Scaled-size Rhodopsin Protein)
Summary

- Interconnects effect to LAMMPS performance
  - InfiniBand enables higher performance/scalability
  - Ethernet provides only 30% scalability at 14 nodes

- Intel Compilers and MKL Libraries can increase single-node performance by 46%

- Running multiple jobs per day, can increase LAMMPS productivity by 6%

- MPI_Send, MPI_Allreduce and MPI_Waitany mostly used MPI calls

- Majority of communication time is spent on MPI_Send and MPI_Allreduce

- Message with sizes around 64B and 64KB mostly used
Thank You
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