LAMMPS-KOKKOS
Performance Benchmark and Profiling

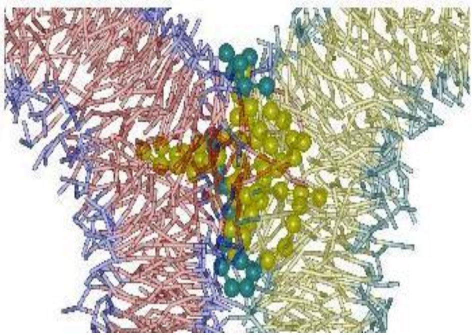
September 2015

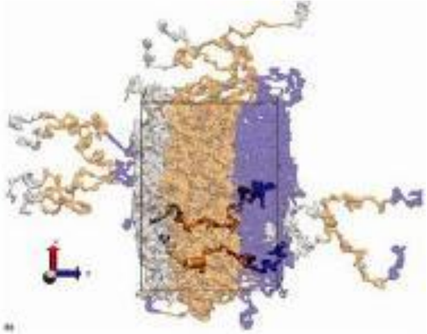
Note

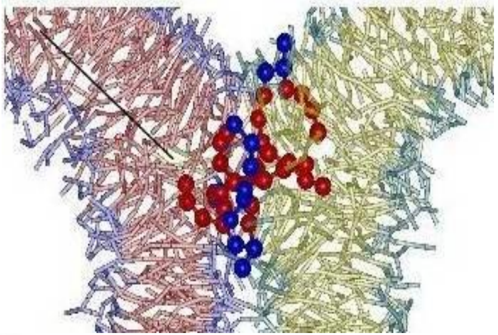
- **The following research was performed under the HPC Advisory Council activities**
  - Participating vendors: Intel, Dell, Mellanox, NVIDIA
  - Compute resource - HPC Advisory Council Cluster Center
- **The following was done to provide best practices**
  - LAMMPS performance overview
  - Understanding LAMMPS communication patterns
  - Ways to increase LAMMPS productivity
- **For more info please refer to**
  - http://lammps.sandia.gov
  - http://www.dell.com
  - http://www.intel.com
  - http://www.mellanox.com
  - http://www.nvidia.com

LAMMPS

- **Large-scale Atomic/Molecular Massively Parallel Simulator**
  - Classical molecular dynamics code which can model:
  - Atomic, Polymeric, Biological, Metallic, Granular, and coarse-grained systems
- **LAMMPS-KOKKOS package contains**
  - Versions of pair, fix, and atom styles that use data structures and macros provided by the Kokkos library
- **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 presented research was done to provide best practices**
  - LAMMPS performance benchmarking
    - MPI Library performance comparison
    - Interconnect performance comparison
    - CPUs comparison
    - Optimization tuning
- **The presented results will demonstrate**
  - The scalability of the compute environment/application
  - Considerations for higher productivity and efficiency

Test Cluster Configuration

- **Dell PowerEdge R730 32-node (896-core) “Thor” cluster**
  - Dual-Socket 14-Core Intel E5-2697v3 @ 2.60 GHz CPUs (BIOS: Maximum Performance, Home Snoop)
  - Memory: 64GB memory, DDR4 2133 MHz, Memory Snoop Mode in BIOS sets to Home Snoop
  - OS: RHEL 6.5, MLNX_OFED_LINUX-3.0-1.0.1 InfiniBand SW stack
  - Hard Drives: 2x 1TB 7.2 RPM SATA 2.5” on RAID 1
- **Mellanox ConnectX-4 EDR 100Gb/s InfiniBand Adapters**
- **Mellanox Switch-IB SB7700 36-port EDR 100Gb/s InfiniBand Switch**
- **Mellanox ConnectX-3 FDR VPI InfiniBand and 40Gb/s Ethernet Adapters**
- **Mellanox SwitchX-2 SX6036 36-port 56Gb/s FDR InfiniBand / VPI Ethernet Switch**
- **Dell InfiniBand-Based Lustre Storage based on Dell PowerVault MD3460 and Dell PowerVault MD3420**
- **NVIDIA Tesla K40 (on 8 Nodes) and NVIDIA Tesla K80 GPUs (on 2 Nodes); 1 GPU per node**
- **MPI: Mellanox HPC-X v1.3 (based on Open MPI 1.8.7) with CUDA 6.5 and 7.0 support**
- **Application: LAMMPS 15May15**
- **Benchmarks: Input data with embedded-atom method (in.eam)**

PowerEdge R730
Massive flexibility for data intensive operations

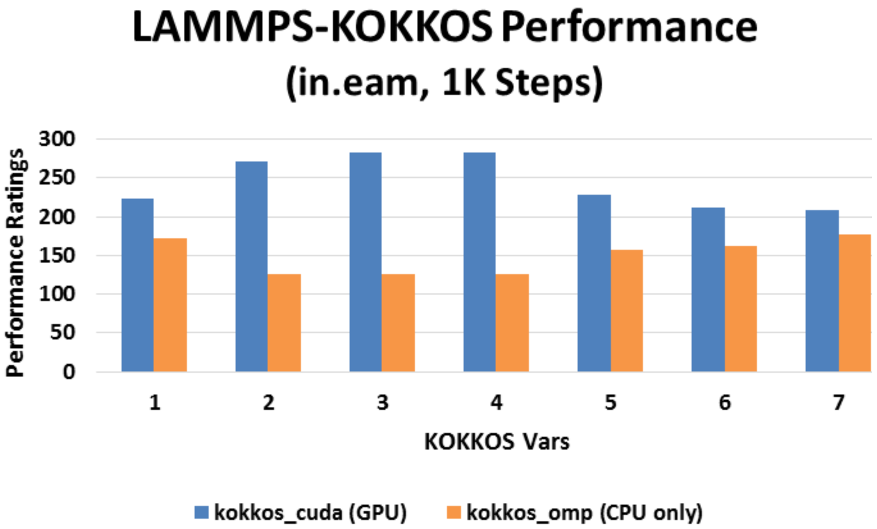
- **Performance and efficiency**
  - Intelligent hardware-driven systems management with extensive power management features
  - Innovative tools including automation for parts replacement and lifecycle manageability
  - Broad choice of networking technologies from Ethernet to InfiniBand
  - Built in redundancy with hot plug and swappable PSU, HDDs and fans

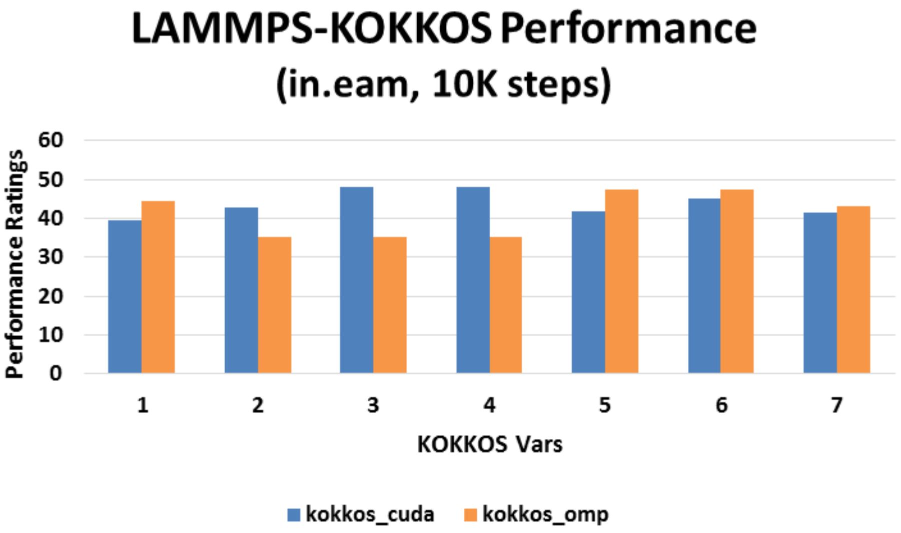
- **Benefits**
  - Designed for performance workloads
  - High performance scale-out compute and low cost dense storage in one package

- **Hardware Capabilities**
  - Flexible compute platform with dense storage capacity
    - 2S/2U server, 6 PCIe slots
  - Large memory footprint (Up to 768GB / 24 DIMMs)
  - High I/O performance and optional storage configurations
    - HDD options: 12 x 3.5” - or - 24 x 2.5 + 2x 2.5 HDDs in rear of server
    - Up to 26 HDDs with 2 hot plug drives in rear of server for boot or scratch

LAMMPS Performance – KOKKOS Vars

- **Kokkos variable determines the communication models between host and device**
  - The best of kokkos vars used for CPU and GPU tests are different
  - The most favorite kokkos vars for GPU appears to be among #2, 3, or 4
  - The most favorite kokkos vars for CPU appears to be among #1, 5, 6, or 7

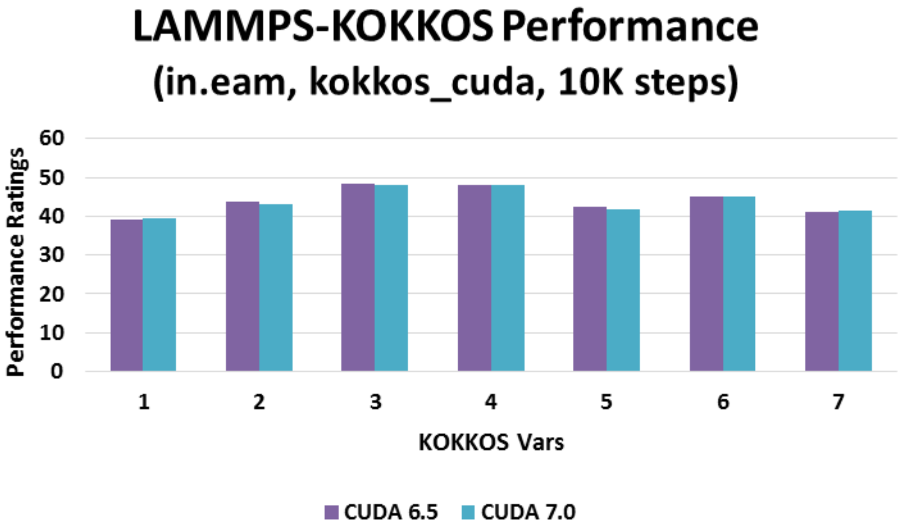




Higher is better

LAMMPS Performance – CUDA Versions

- **Both CUDA 6.5 and 7.0 versions perform similarly**
  - Using the given input data and workload

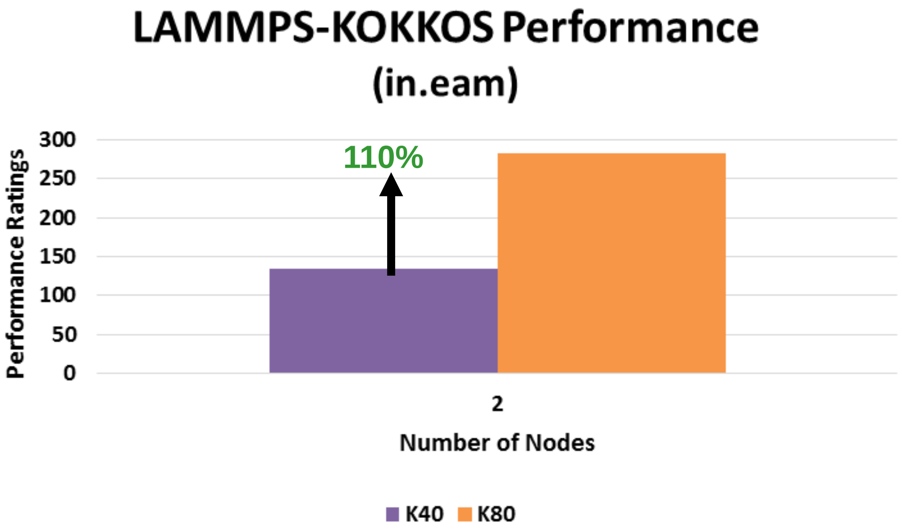


Higher is better

8 Nodes; 1x K40 / Node

LAMMPS Performance – Tesla K40 vs K80

- **Tesla K80 doubles the performance of K40 using with LAMMPS**
  - Demonstrates 110% increase in performance on 2 nodes with 1 GPU per node

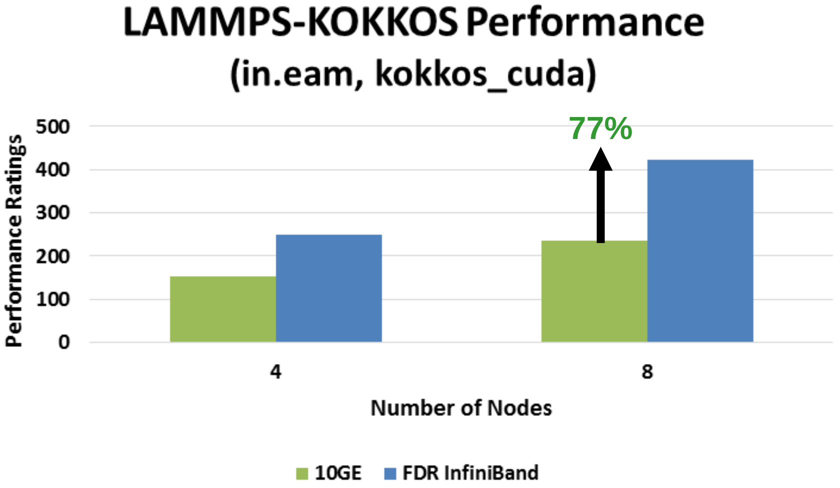


Higher is better

1 GPU / Node

LAMMPS Performance – Network Interconnects

- **EDR InfiniBand delivers superior scalability in application performance**
  - InfiniBand delivers 77% higher performance than 10GbE on 8 nodes
- **Performance of 4 IB nodes outperforms 8 Ethernet (10GbE) nodes**
  - Benefits of InfiniBand over Ethernet expect to increase as cluster scales
  - Scalability for Ethernet stops beyond 4 nodes; while InfiniBand continue to scale

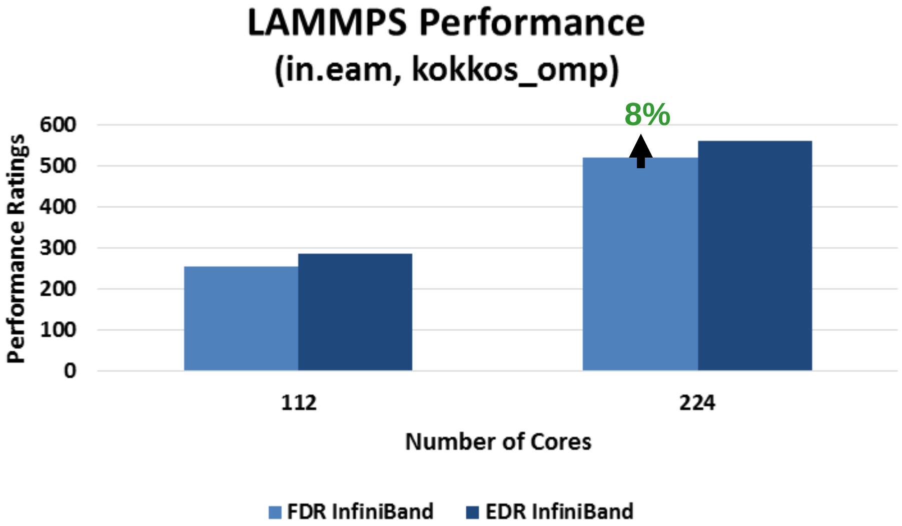


Higher is better

GPU: 1 K40 / Node

LAMMPS Performance – Network Interconnects

- **EDR InfiniBand delivers superior scalability in application performance**
  - EDR IB demonstrates an 8% increase on 8 Nodes / 224 Cores
  - Performance gap between FDR and EDR expect to increase as cluster scales

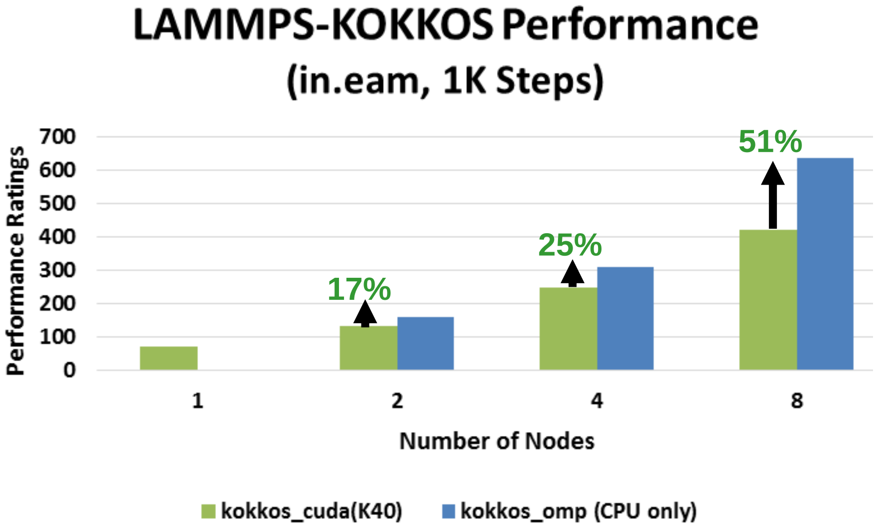


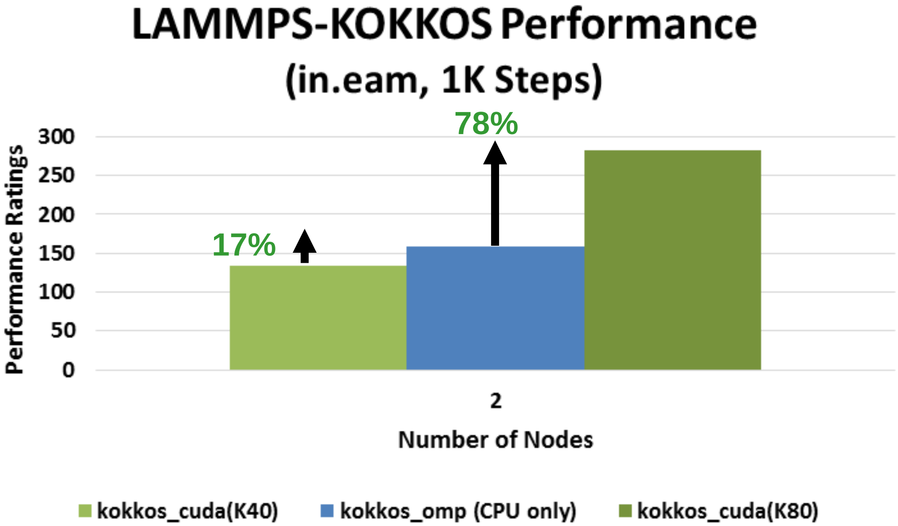
Higher is better

28 MPI Processes / Node

LAMMPS Performance – Scalability

- **kokkos_omp demonstrates higher speed up and performance than kokkos_cuda**
  - CPU performance outpaces Tesla K40 performance using 28 cores/node
  - With the availability of the Tesla K80, it outperforms CPU; performance gap expect to grow





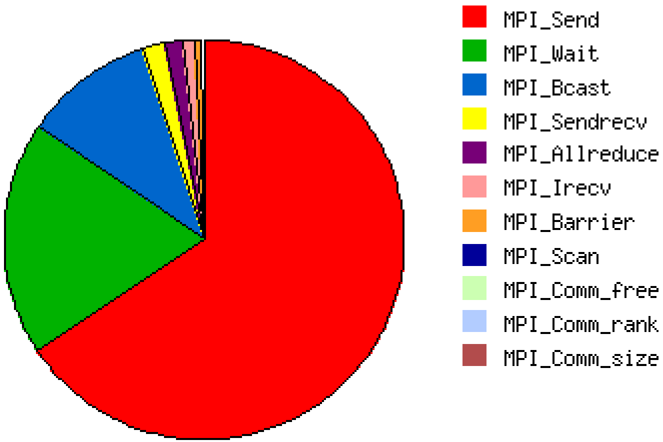
CPU: 28 Processes/Node
GPU: 1 GPU / Node

Higher is better

LAMMPS Profiling – % of MPI Calls

- **The most time consuming MPI calls for LAMMPS-KOKKOS (cuda):**
  - MPI_Send: 67% MPI / 8% Wall
  - MPI_Wait: 18% MPI / 2% Wall
  - MPI_Bcast: 11% MPI / 1% Wall

Kokkos_cuda, 8 nodes / 224 processes

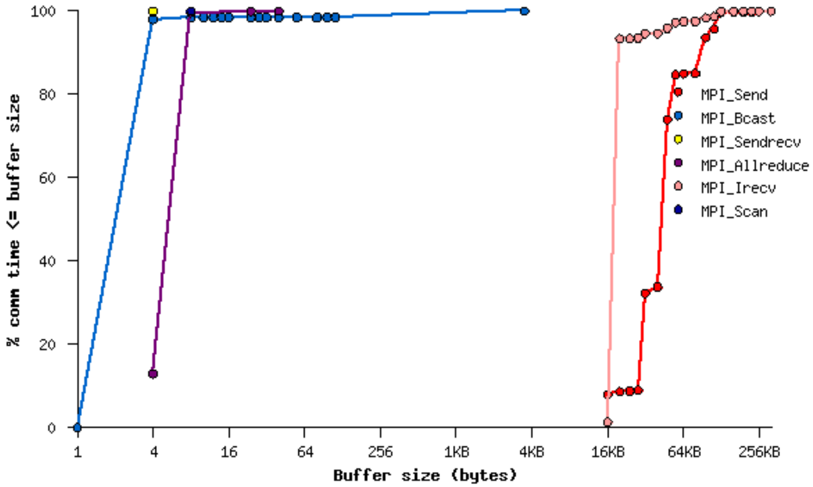


EDR InfiniBand

LAMMPS Profiling – MPI Message Size Distribution

- **For the most time consuming MPI calls**
  - MPI_Send: 48KB (26% MPI) time, 32KB (15%), 56KB (7%)
  - MPI_Wait: 0B (18% MPI time)
  - MPI_Bcast: 4B (10% MPI time)

Kokkos_cuda, 8 nodes / 224 processes

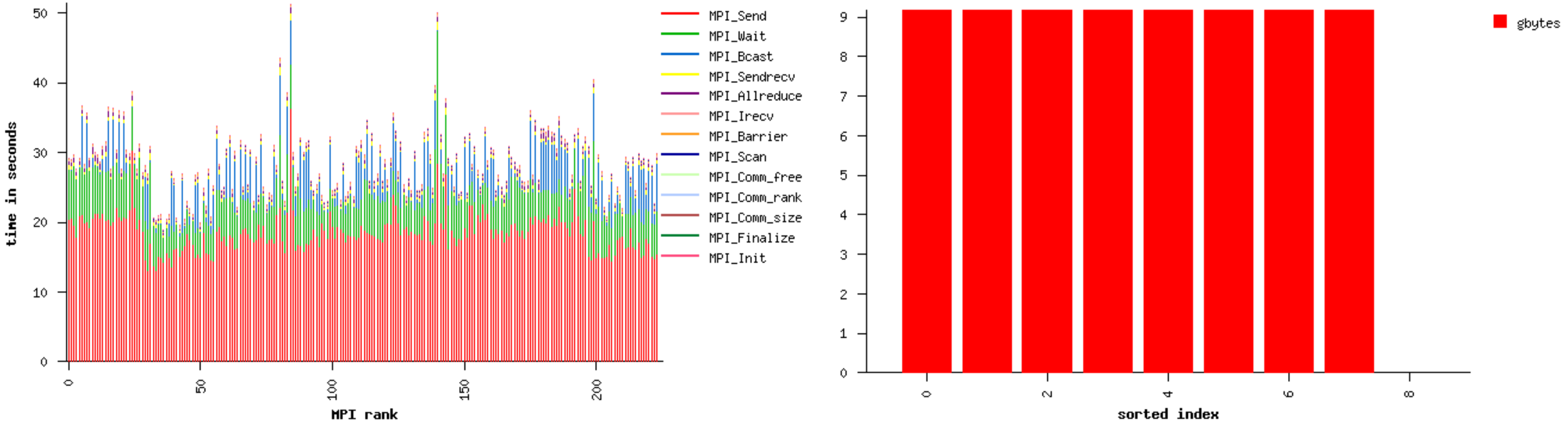


EDR InfiniBand

LAMMPS Profiling – MPI Memory Consumption

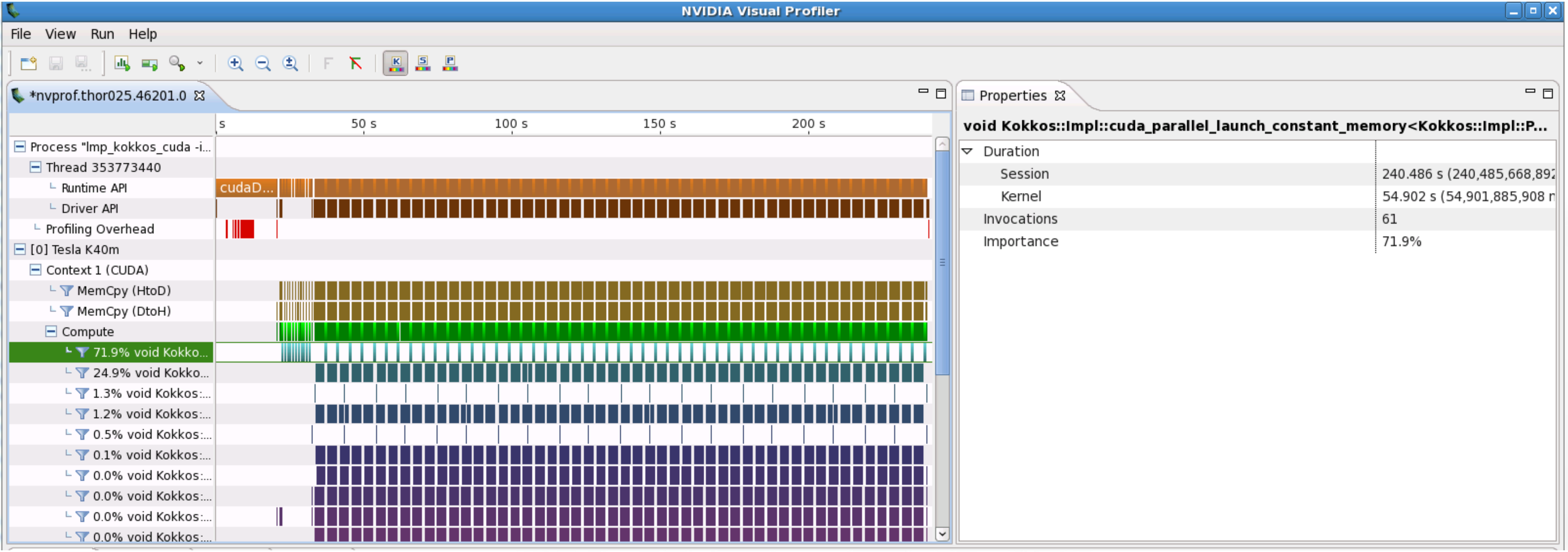
- **Some load imbalance is seen on the processes**
- **Memory consumption:**
  - About 9GB of memory is used on each compute node for this input data

Kokkos_cuda, 8 nodes / 224 processes



LAMMPS Profiling – CUDA Profiler

- **NVIDIA Visual Profiler and nvprof: Profilers for GPUs**
  – Shows many Memcpy occurs between host and device throughout the run



void Kokkos::Impl::cuda_parallel_launch_constant_memory<Kokkos::Impl::P...

Duration	
Session	240.486 s (240,485,668,892
Kernel	54.902 s (54,901,885,908 n
Invocations	61
Importance	71.9%

LAMMPS Summary

- **Performance**
  - Compute: cluster of the current generation outperforms system architecture of previous generations
    - Tesla K80 doubles the performance of K40 using with LAMMPS-KOKKOS
    - The KOKKOS vars can be a significant performance implication to the performance of LAMMPS
    - CUDA versions 6.5 and 7.0 performs similarly
  - Network: EDR InfiniBand demonstrates superior scalability in LAMMPS performance
    - EDR IB provides higher performance by 77% over 10GbE, 86% higher over 1GbE on 8 nodes
    - Performance of 4 IB nodes outperforms 8 Ethernet (10GbE) nodes
    - Benefits of InfiniBand over Ethernet expect to increase as cluster scales
    - Scalability for Ethernet stops beyond 4 nodes; while InfiniBand continue to scale
  - MPI Profiles
    - The most time consuming MPI calls for LAMMPS-KOKKOS (cuda):
    - MPI_Send: 67% MPI / 8% Wall
    - MPI_Wait: 18% MPI / 2% Wall
    - MPI_Bcast: 11% MPI / 1% Wall

Thank You

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