# GROMACS
# Performance Benchmark and Profiling

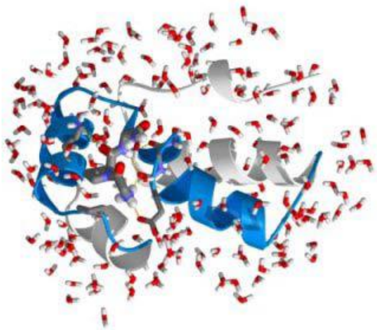
July 2015

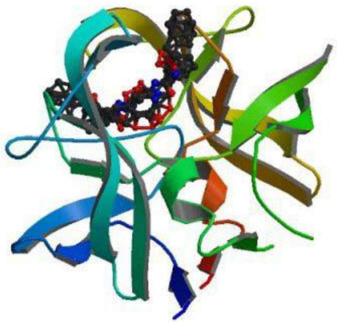
# Note

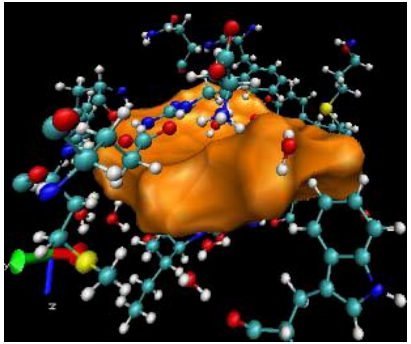
- **The following research was performed under the HPC Advisory Council activities**
  - Participating vendors: Intel, Dell, Mellanox
  - Compute resource - HPC Advisory Council Cluster Center
- **The following was done to provide best practices**
  - GROMACS performance overview
  - Understanding GROMACS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

# GROMACS

- **GROMACS (GROningen MAchine for Chemical Simulation)**
  - A molecular dynamics simulation package
  - Primarily designed for biochemical molecules like proteins, lipids and nucleic acids
    - A lot of algorithmic optimizations have been introduced in the code
    - Extremely fast at calculating the nonbonded interactions
  - Ongoing development to extend GROMACS with interfaces both to Quantum Chemistry and Bioinformatics/databases
  - An open source software released under the GPL







# Objectives

- **The presented research was done to provide best practices**
  - GROMACS performance benchmarking
    - CPU performance comparison
    - MPI library performance comparison
    - Interconnect performance comparison
    - System generations comparison
- **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 (Power Management in BIOS sets to Maximum Performance)
  - Memory: 64GB memory, DDR4 2133 MHz, Memory Snoop Mode in BIOS sets to Home Snoop, Turbo Enabled
  - 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 100Gbps EDR InfiniBand Adapters**
- **Mellanox Switch-IB SB7700 36-port 100Gb/s EDR InfiniBand Switch**
- **Mellanox ConnectX-3 FDR InfiniBand, 10/40GbE Ethernet VPI Adapters**
- **Mellanox SwitchX-2 SX6036 36-port 56Gb/s FDR InfiniBand / VPI Ethernet Switch**
- **MPI: Mellanox HPC-X v1.2.0-326**
- **Compiler and Libraries: Intel Composer XE 2015.3.187 and MKL**
- **Application: GROMACS 4.6.7**
- **Benchmark datasets: DPPC in Water (d.dppc, 121856 atoms, 150000 steps, SP) unless stated otherwise**

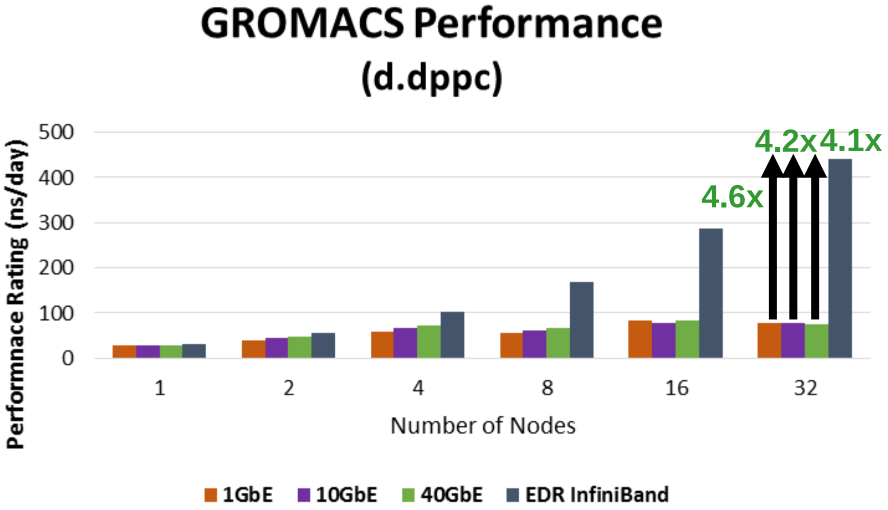
# PowerEdge R730

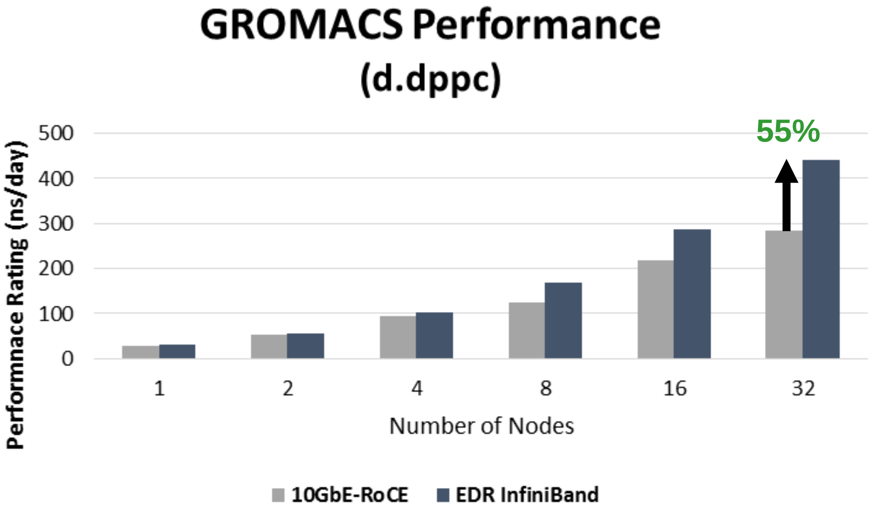
## Massive flexibility for data intensive operations

- **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 GigE to IB
  - Built in redundancy with hot plug and swappable PSU, HDDs and fans
- **Benefits**
  - Designed for performance workloads
    - from big data analytics, distributed storage or distributed computing where local storage is key to classic HPC and large scale hosting environments
    - 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

# GROMACS Performance – Network Interconnects

- **InfiniBand is the only interconnect that delivers superior scalability performance**
  - EDR InfiniBand provides higher performance and more scalable than 1GbE, 10GbE, or 40GbE
  - Performance for Ethernet stays flat (or stops scaling) beyond 2 nodes
  - EDR InfiniBand outperforms 10GbE-RoCE on scalability performance by 55% at 32 nodes / 896c
  - EDR InfiniBand demonstrates continuous performance gain at scale



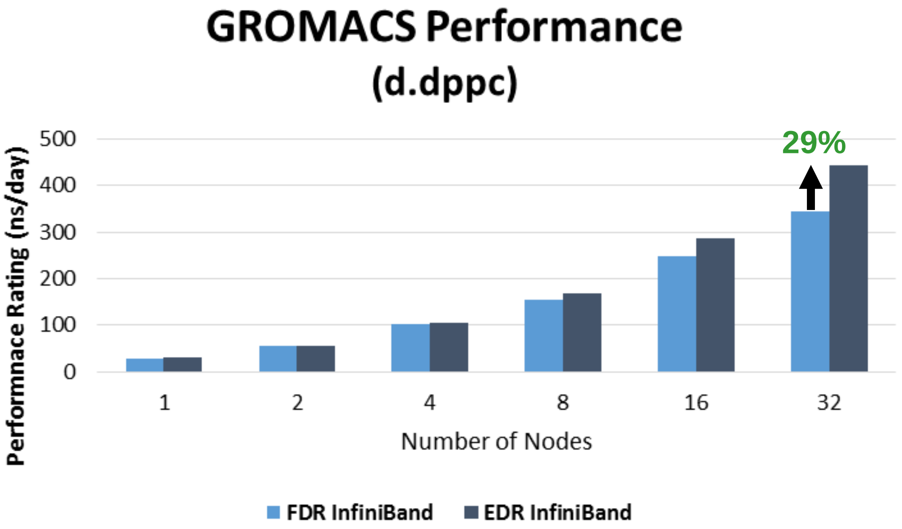


*Higher is better*

*28 MPI Processes / Node*

# GROMACS Performance – EDR vs FDR InfiniBand

- **EDR InfiniBand delivers superior scalability in application performance**
  - As the number of nodes scales, performance gap of EDR IB becomes widen
- **Performance advantage of EDR InfiniBand increases for larger core counts**
  - EDR InfiniBand provides 29% versus FDR InfiniBand at 32 nodes (896 cores)

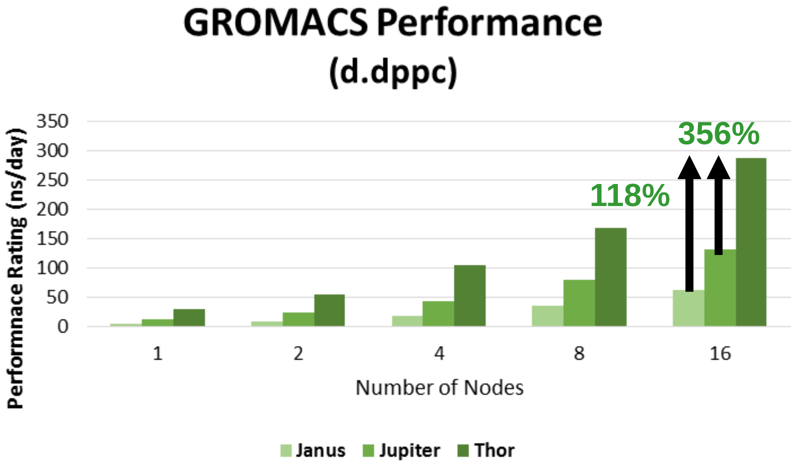


*Higher is better*

*28 MPI Processes / Node*

# GROMACS Performance – System Generations

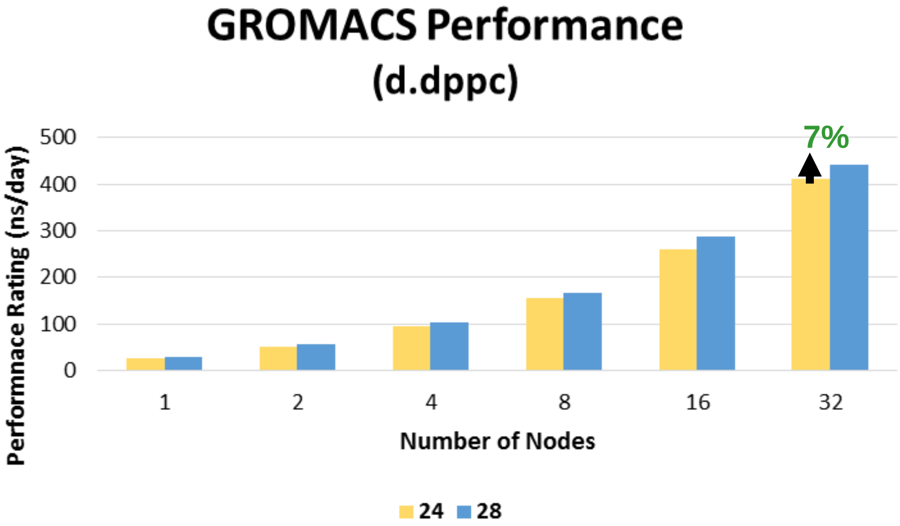
- **Thor cluster (based on Intel E5-2697v3 - Haswell) outperforms prior generations**
  - 1.1 to 3.5x higher performance than clusters based on previous generations of Intel architecture
- **System components used:**
  - Janus: 2-socket 6-core Xeon X5670 @ 2.93GHz, 1333MHz DIMMs, ConnectX-2 QDR IB
  - Jupiter: 2-socket 8-core Xeon E5-2680 @ 2.7GHz, 1600MHz DIMMs, ConnectX-3 FDR IB
  - Thor: 2-socket 14-core Xeon E5-2680V3 @2.6GHz, 2133MHz DIMMs, ConnectX-4 EDR IB



*Higher is better*

# GROMACS Performance – Cores Per Node

- **Running more CPU cores provides higher performance**
  - ~7-10% higher productivity with 28PPN compared to 24PPN
  - Higher demand on memory bandwidth and network might limit performance as more cores are used

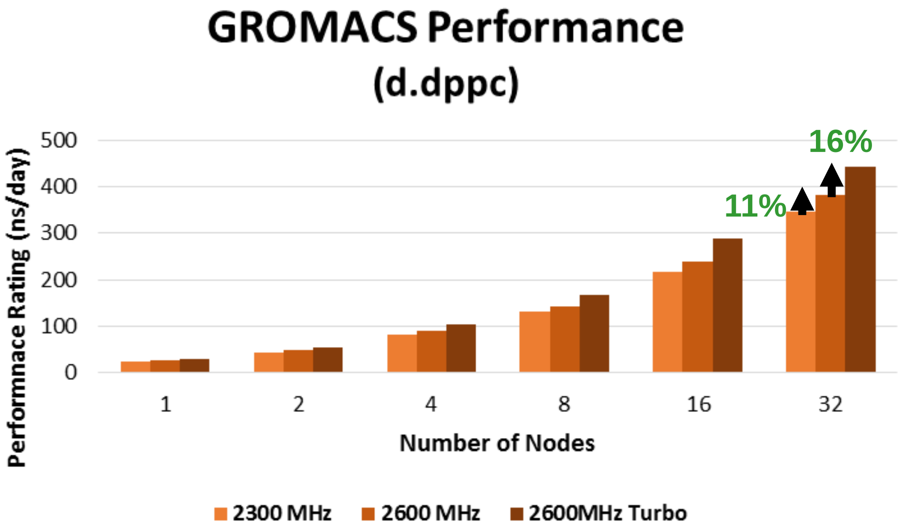


*Higher is better*

*CPU @ 2.6GHz*

# GROMACS Performance – Turbo Mode & CPU Clock

- **Advantages are seen with running higher clock rate**
  - Either by enabling Turbo mode or higher CPU clock frequency
- **Boosting CPU clock rate yields higher performance at lower cost**
  - Increasing to 2600MHz (from 2300MHz) run 11% faster

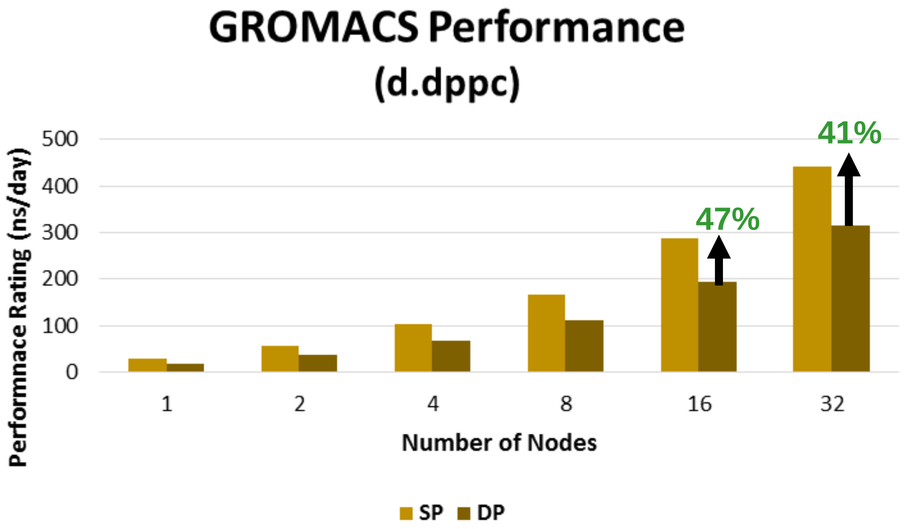


*Higher is better*

*CPU @ 2.6GHz*

# GROMACS Performance – Floating Point Precision

- **GROMACS allows running either SP and DP for floating point precision**
- **Running at SP is shown to be faster than running at DP**
  - Seen around 41%-47% faster running at SP (Single Precision) versus DP (Double Precision)
  - All other slides are running using Single Precision

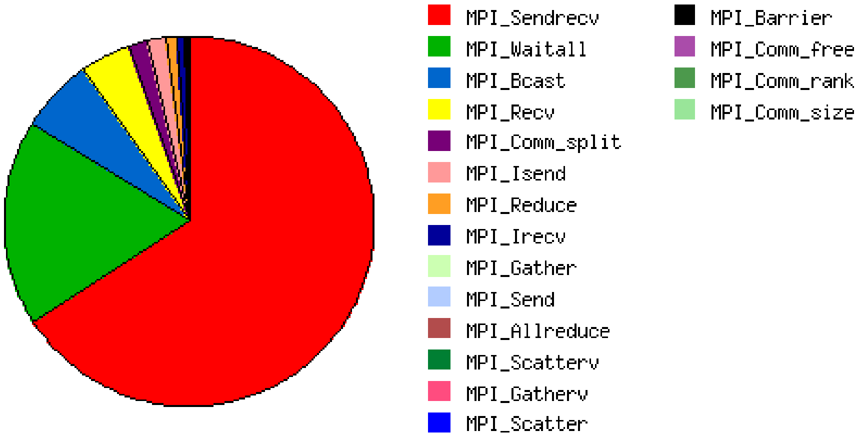


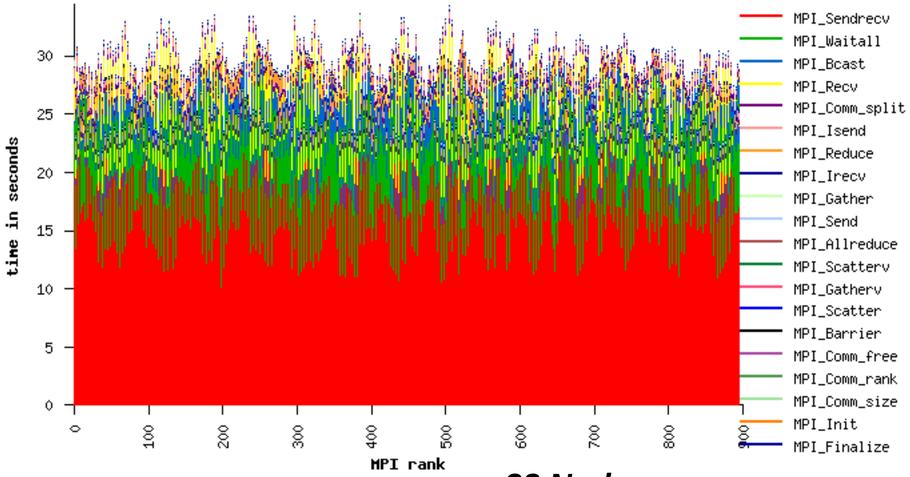
*Higher is better*

*CPU @ 2.6GHz*

# GROMACS Profiling – Time Spent by MPI Calls

- **The most time consuming MPI call os MPI_Sendrecv**
  - MPI_Sendrecv: 66% (or 27% of runtime) at 32 nodes (896 cores)
  - MPI_Waitall: 18% (or 7% of runtime), MPI_Bcast: 6% (or 2% of runtime)
  - Point to point and non-blocking sends and receives consume most time in GROMACS

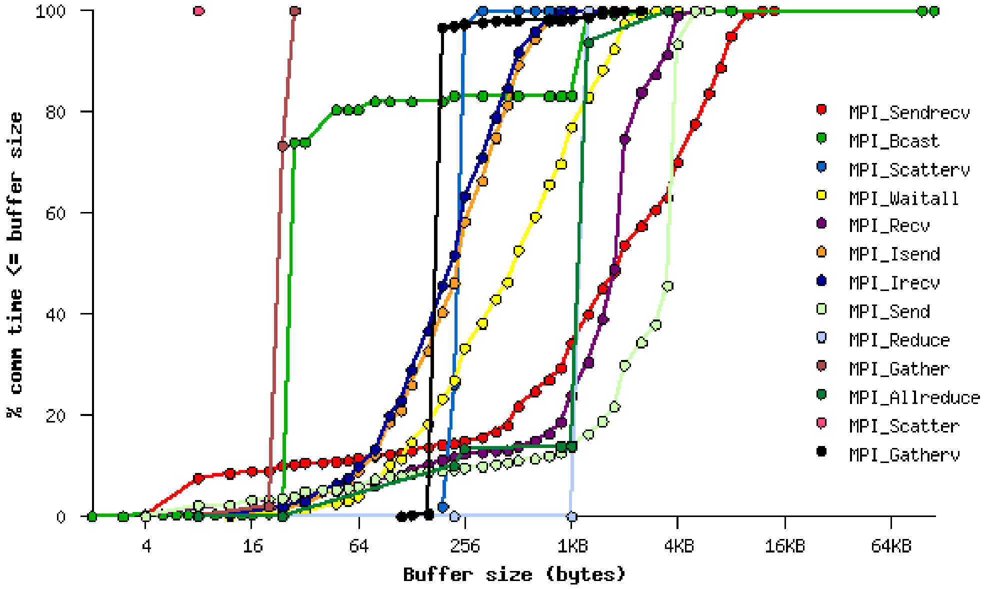




***32 Nodes***

# GROMACS Profiling – MPI Message Sizes

- **Majority of data transfer messages are medium sizes, except for:**
  - MPI_Sendrecv has a large concentration (from 8B to 8KB)
  - MPI_Bcast shows some concentration

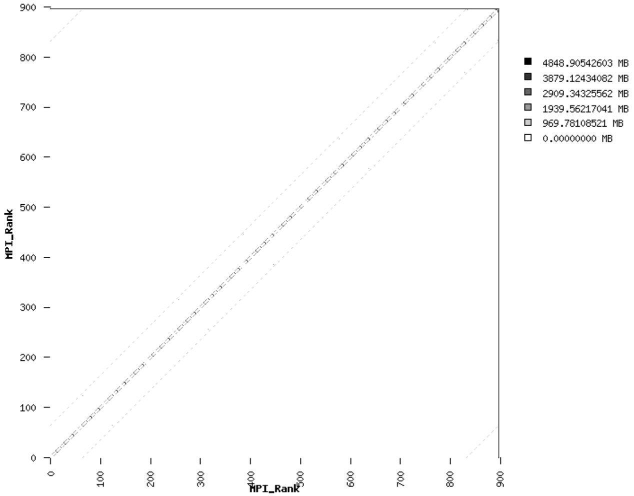


***32 Nodes***

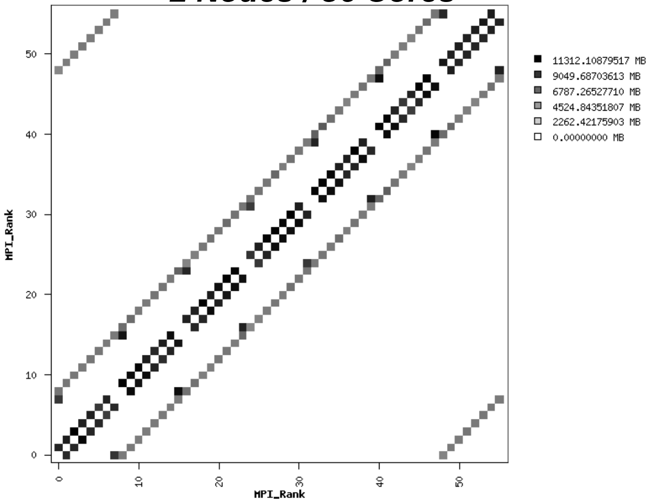
# GROMACS Profiling – MPI Data Transfer

- **As the cluster grows, similar communication behavior is seen**
  - Majority of communications are between neighboring ranks
  - Non-blocking (point to point) data, and point-to-point transfers are shown in the graph
  - Collective data communications are small compared to point-to-point communications

***32 Nodes / 896 Cores***



***2 Nodes / 56 Cores***



# GROMACS Summary

- **Latest system generation improve GROMACS performance at scale**
  - Compute: Intel Haswell cluster outperforms system architecture of previous generations
    - Haswell cluster outperforms Sandy Bridge cluster by 110%, and outperforms Westmere cluster by 350% at 32 node
  - Compute: Running more CPU cores provides higher performance
    - ~7-10% higher productivity with 28PPN compared to 24PPN
  - Network: EDR InfiniBand delivers superior scalability in application performance
    - EDR InfiniBand provides higher performance and more scalable than 1GbE, 10GbE, or 40GbE
    - Performance for Ethernet (1GbE/10GbE/40GbE) stays flat (or stops scaling) beyond 2 nodes
    - EDR InfiniBand outperforms 10GbE-RoCE on scalability performance by 55% at 32 nodes / 896c
  - Running at Single Precision is approximately twice as fast as running at Double Precision
    - Seen around 41%-47% faster running at SP (Single Precision) versus DP (Double Precision)
  - MPI Profile shows majority of data transfer are point-to-point and non-blocking communications
    - MPI_Sendrecv and MPI_Waitall are the most used MPI communication

# Thank You

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