



NAMD Performance Benchmark and Profiling

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- The following research was performed under the HPC Advisory Council activities
 - Participating vendors: AMD, Dell, Mellanox
 - Compute resource HPC Advisory Council Cluster Center
- For more info please refer to
 - http:// www.amd.com
 - <u>http:// www.dell.com/hpc</u>
 - 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



Theoretical and Computational Biophysics Group Beckman Institute University of Illinois at Urbana-Champaign





Objectives



The following was done to provide best practices

- NAMD performance benchmarking
- Interconnect performance comparisons
- Ways to increase NAMD productivity
- MPI libraries comparisons

The presented results will demonstrate

- The scalability of the compute environment to provide nearly linear application scalability
- The capability of NAMD to achieve scalable productivity
- Considerations for performance optimizations

Test Cluster Configuration



- Dell[™] PowerEdge[™] R815 11-node (704-core) cluster
- AMD[™] Opteron[™] 6276 (code name "Interlagos") 16-core @ 2.3 GHz CPUs
- 4 CPU sockets per server node
- Mellanox ConnectX®-3 FDR InfiniBand Adapters
- Mellanox SwitchX[™] 6036 36-Port InfiniBand switch
- Memory: 128GB memory per node DDR3 1333MHz
- OS: RHEL 6.2, MLNX-OFED 1.5.3 InfiniBand SW stack
- MPI: Open MPI 1.5.5rc2, Platform MPI 8.2
- Compilers: GNU Compilers 4.6
- Application: NAMD 2.8 (External libraries used: charm-6.2.3, fftw-2.1.3, TCL 8.3)
- Benchmark workload:
 - ApoA1 bloodstream lipoprotein particle model (92,224 atoms, periodic, PME, 12A cutoff)
 - ATPase benchmark (327,506 atoms, periodic, PME)

Dell[™] PowerEdge[™] R815 11-node cluster



HPC Advisory Council Test-bed System

• New 11-node 704 core cluster - featuring Dell PowerEdge™ R815 servers

- Replacement system for Dell PowerEdge SC1435 (192 cores) cluster system following 2 years of rigorous benchmarking and product EOL
 - System to be redirected to explore HPC in the Cloud applications

Workload profiling and benchmarking

- Characterization for HPC and compute intense environments
- Optimization for scale, sizing and configuration and workload performance
- Test-bed Benchmarks
 - RFPs
 - Customers/Prospects, etc
- ISV & Industry standard application characterization
- Best practices & usage analysis



About Dell PowerEdge[™] Platform Advantages



Best of breed technologies and partners

Combination of AMD Opteron[™] 6200 series platform and Mellanox ConnectX®-3 InfiniBand on Dell HPC

Solutions provide the ultimate platform for speed and scale

- Dell PowerEdge R815 system delivers 4 socket performance in dense 2U form factor
- Up to 64 core/32DIMMs per server 1344 core in 42U enclosure

Integrated stacks designed to deliver the best price/performance/watt

- 2x more memory and processing power in half of the space
- Energy optimized low flow fans, improved power supplies and dual SD modules

Optimized for long-term capital and operating investment protection

- System expansion
- Component upgrades and feature releases



NAMD Performance – Processors



- Interlagos CPUs provides better performance than Magny-Cours CPUs
 - Up to 34% gain in performance with Open MPI versus Magny-Cours CPUs
- Processors used:
 - Magny-Cours: AMD Opteron[™] 6174 (2200MHz)
 - Interlagos: AMD Opteron[™] 6276 (2300MHz)



NAMD Performance

(Apoa1, Open MPI)

Higher is better

64 Cores/Node

NAMD Performance – Interconnects



- InfiniBand enables better scalability for NAMD
 - Showing unlimited continuous gain to 7-node
- Ethernet does not allow good scalability
 - The performance of 1GbE plummet after 2 nodes (128 processes)
 - Both 1GbE and 10GbE do not show gain in productivity
 - The effect of MPI communications overwhelms the Ethernet network



NETWORK OF EXPERTISE

NAMD Performance – Open MPI Tuning



Using XRC in Open MPI allows better performance and scalability

- Stands for eXtended Reliable Connection
- Reduces memory footprint and is essential for scaling
- Flags used: -mca btl_openib_receive_queues
 X,128,256,192,128:X,2048,256,128,32:X,12288,256,128,32:X,65536,256,128,32
- Open MPI optimization flags used in both cases:
 - bind-to-core -mca btl openib,sm,self



NETWORK OF EXPERTISE

NAMD Performance – Platform MPI Tuning



- Using SRQ (Shared Receive Queue) allow Platform MPI to scale
 - Reduces memory footprint and is essential for scaling
- Explicit mapping of CPU cores to ensure MPI ranks are placed sequentially
 - To ensure CPU core enumeration, check with "Istopo" from hwloc or "numactl --hardware"
- Extra flags in optimized case for SRQ, RDMA params and core bindings:
 - -srq -e MPI_RDMA_MSGSIZE=32768,32768,4194304 -e MPI_RDMA_NSRQRECV=2048 -e MPI_RDMA_NFRAGMENT=128 cpu_bind=v,map_cpu:0,4,8,12,16,20,24,28,32,36,40,44,48,52,56,60,2,6,10,14,18,22,26,30,34,38,42,46,50,54,58,62,3,7,11,15,19,23,27,31,35,39 ,43,47,51,55,59,63,1,5,9,13,17,21,25,29,33,37,41,45,49,53,57,61



NAMD Performance – MPI Implementations



- The Platform MPI performs better than Open MPI
 - Up to 8% better than Open MPI for apoa1 at 7-node
 - Up to 13% better than Open MPI for f1atpase at 7-node
- The tuned flags are used for both Platform MPI and Open MPI



NAMD Profiling – MPI/User Time Ratio



- NAMD becomes highly communicative starting from 2-3 nodes
 - Due to the high core counts per node
 - The stmv contains more CPU and MPI communication times than apoa1
- MPI communication time dominates the overall time
 - Shows low latency interconnect such as InfiniBand is required for good scalability



NETWORK OF EXPERTISE

NAMD Profiling – Number of MPI Calls



- The most used MPI function is MPI_Iprobe
 - MPI_Iprobe is used for testing non-blocking messages
 - Accounted for 97% of all MPI calls



NAMD Profiling – MPI Message Sizes



- Majority of the MPI message sizes are
 - in the range from 4KB to 16KB
- The increase in messages accelerates starting around 5-6 nodes



NAMD Profiling – Data Transfer Per Process



- Data transferred to each MPI rank is showing some variance
 - But overall data transfer is roughly the same on a per-node basis
- As the cluster scales, less data is driven to each rank and each node
 - 300-600MB per rank in 1-node job versus 150-200MB per rank in a 4-node job



NAMD Profiling – Aggregated Data Transfer



- Aggregated data transfer refers to:
 - Total amount of data being transferred in the network between all MPI ranks collectively
- The total data transfer increases as the cluster scales
- Demonstrates the importance of scalable network interconnect
 - InfiniBand can deliver bandwidth needed to push data in 40GB+ across the network



Summary



- Interlagos provides higher performance than Magny-Cours CPUs
 - Up to 34% performance gain with Open MPI
 - AMD Opteron[™] 6276 (code name "Interlagos") 16-core @ 2.3 GHz CPUs
 - AMD Opteron[™] 6174 (code name "Magny-Cours") 12-core @ 2.2GHz CPUs
- Mellanox ConnectX®-3 proves significantly higher scalability for NAMD
 - 4x to 5x higher performance versus 10GbE
- Open MPI and Platform MPI benefit from tuned parameters
 - Having XRC and SRQ enabled the MPIs to scale at large core counts
- The tuned Platform MPI performs better than the tuned Open MPI
 - By 8-13% on 2 different datasets



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