Scheduling Strategies for HPC as a Service (HPCaaS) for Bio-Science Applications

(CPMD, NAMD)

March 2009

AMD
The future is fusion

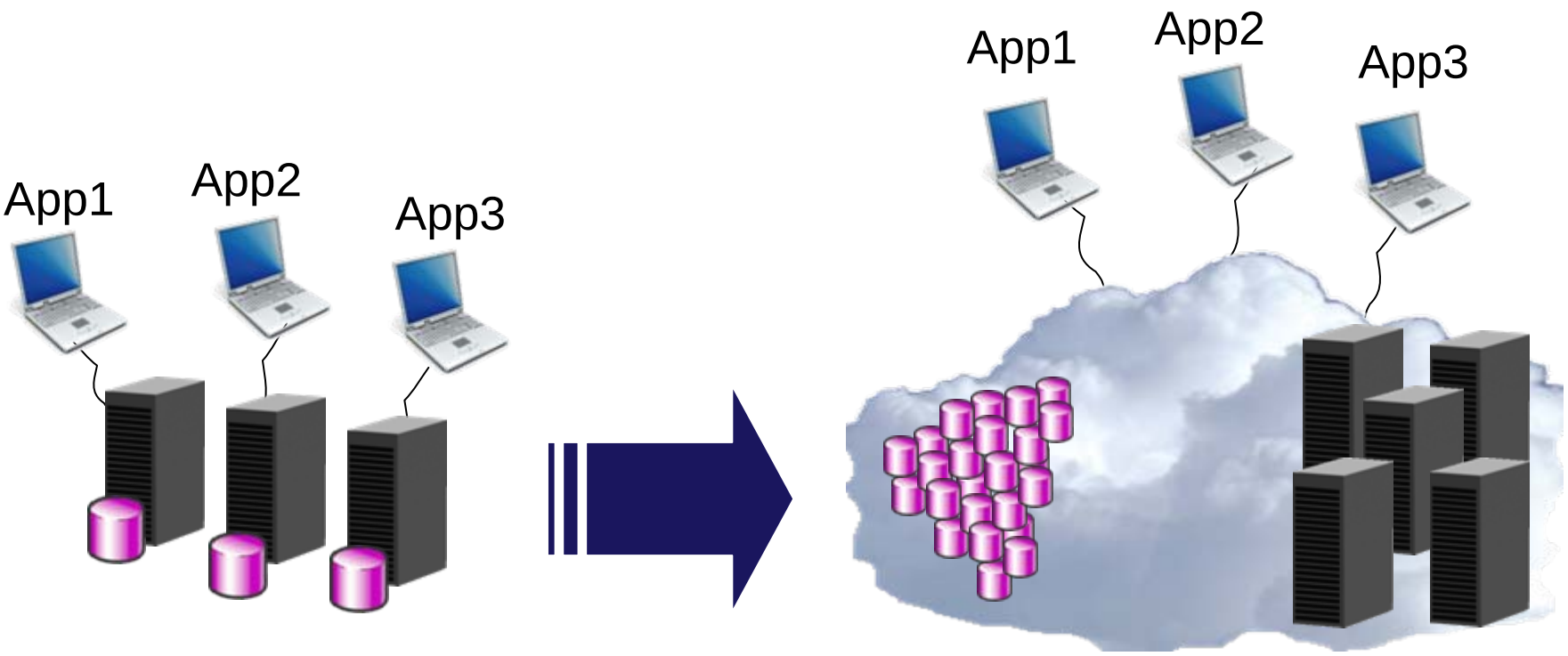
DELL

Mellanox
TECHNOLOGIES

Note

- **The following research was performed under the HPC Advisory Council activities**
  - Special thanks to AMD, Dell, Mellanox Technologies
  - For more info please refer to
    - www.mellanox.com, www.dell.com/hpc, www.amd.com
- **Testing center: HPC Advisory Council Cluster Center**

HPC Centers Evolution



- From equipment warehouse to service provider
- From dedicated HW per application to application services
- Higher productivity, simplicity and efficiency

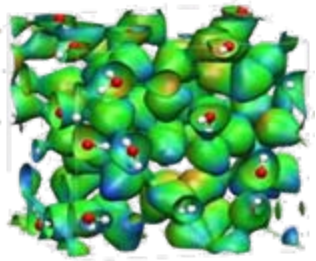
Research Objectives

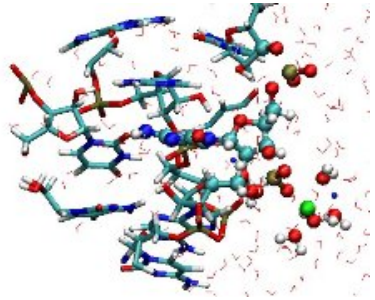
- **Investigate HPC as a Service for bio-science applications**
  - In particular NAMD and CPMD
- **Performance and productivity impact**
- **Cluster interconnect effects on applications performance**

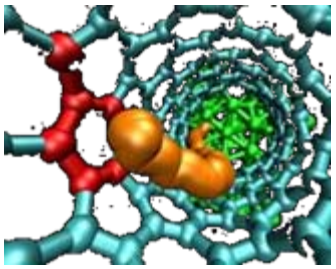
- **For specific information on NAMD and CPMD, please refer to additional studies at**
  - http://hpcadvisorycouncil.mellanox.com/best_practices.php

Car-Parrinello Molecular Dynamics (CPMD)

- **A parallelized implementation of density functional theory (DFT)**
- **Particularly designed for ab-initio molecular dynamics**
- **Brings together methods**
  - Classical molecular dynamics
  - Solid state physics
  - Quantum chemistry
- **CPMD supports MPI and Mixed MPI/SMP**
- **CPMD is distributed and developed by the CPMD consortium**

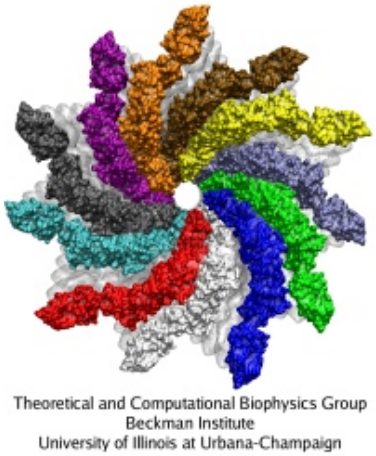


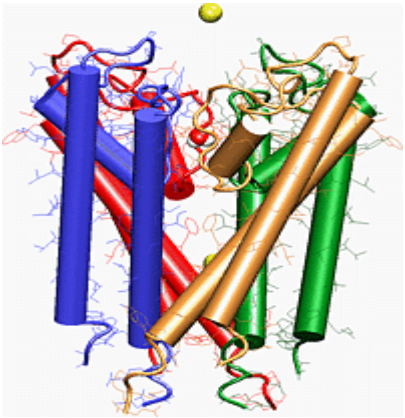


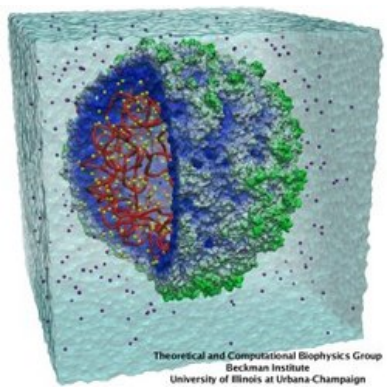


NAMD

- **A parallel, object-oriented molecular dynamics software**
- **Designed for high-performance simulation of large biomolecular systems**
  - 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**







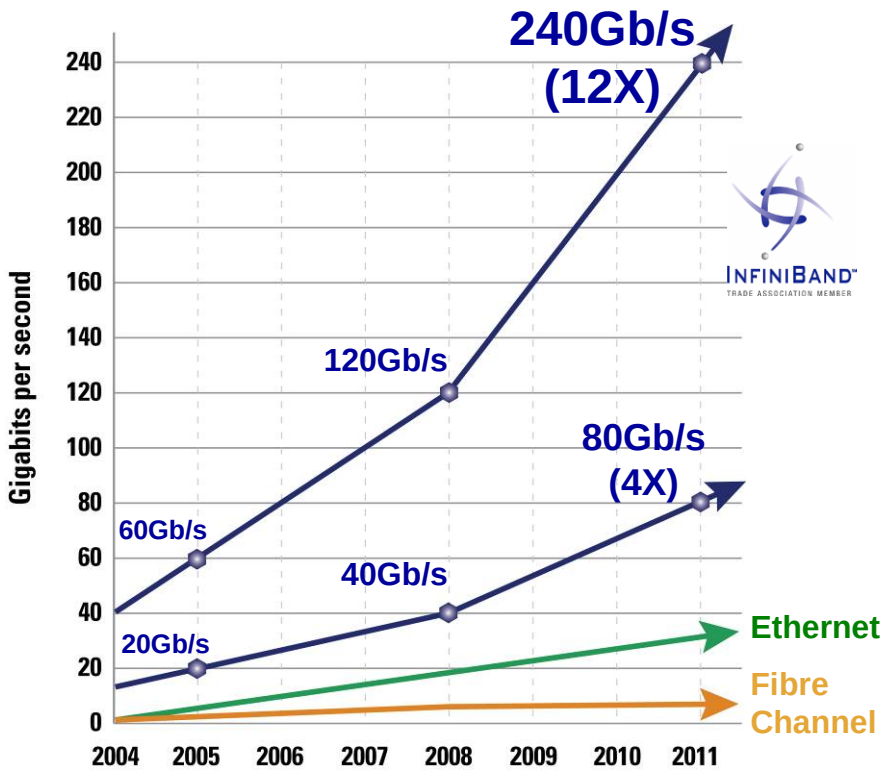
Test Cluster Configuration

- **Dell™ PowerEdge™ SC 1435 24-node cluster**
- **Quad-Core AMD Opteron™ 2382 (“Shanghai”) CPUs**
- **Mellanox® InfiniBand ConnectX® DDR HCAs and InfiniBand DDR Switch**
- **Memory: 16GB memory, DDR2 800MHz per node**
- **OS: RHEL5U2, OFED 1.3 InfiniBand SW stack**
- **MPI: Open MPI 1.3, Platform MPI 5.6.4**
- **Compiler: GCC 4.2.0**
- **Benchmark Application:**
  - CPMD 3.13
    - Benchmark Dataset: C120
  - NAMD 2.6 with fftw3 libraries and Charm++ 6.0
    - Benchmark Dataset: **ApoA1 (92,224 atoms, 12A cutoff)**

Mellanox InfiniBand Solutions

- **Industry Standard**
  - Hardware, software, cabling, management
  - Design for clustering and storage interconnect
- **Performance**
  - 40Gb/s node-to-node
  - 120Gb/s switch-to-switch
  - 1us application latency
  - Most aggressive roadmap in the industry
- **Reliable with congestion management**
- **Efficient**
  - RDMA and Transport Offload
  - Kernel bypass
  - CPU focuses on application processing
- **Scalable for Petascale computing & beyond**
- **End-to-end quality of service**
- **Virtualization acceleration**
- **I/O consolidation Including storage**

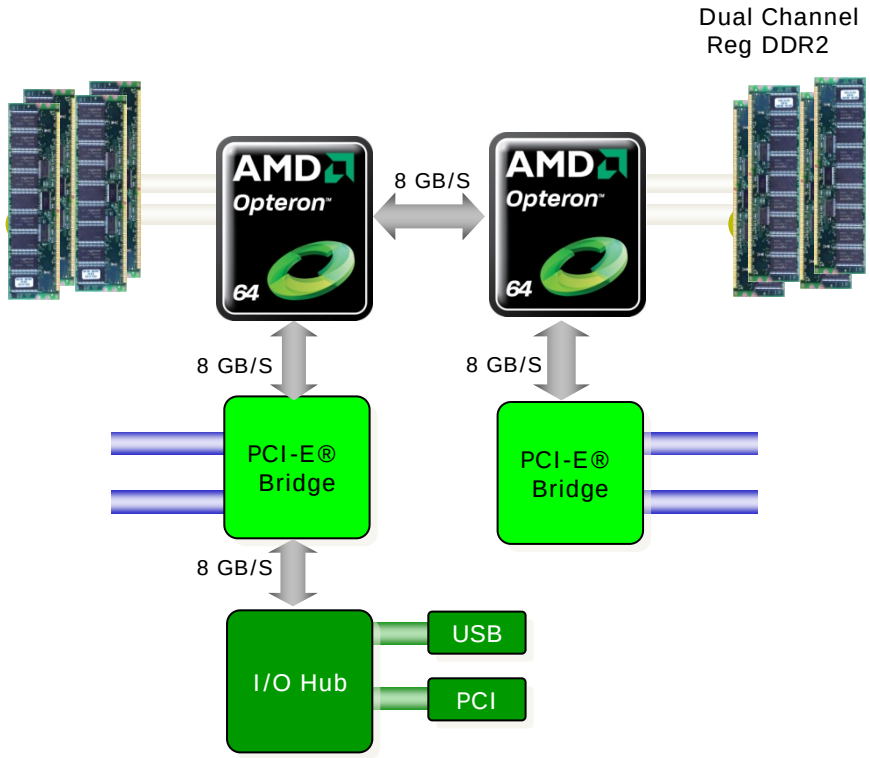
The InfiniBand Performance Gap is Increasing



InfiniBand Delivers the Lowest Latency

Quad-Core AMD Opteron™ Processor

- **Performance**
  - Quad-Core
    - Enhanced CPU IPC
    - 4x 512K L2 cache
    - 6MB L3 Cache
  - Direct Connect Architecture
    - HyperTransport™ Technology
    - Up to 24 GB/s peak per processor
  - Floating Point
    - 128-bit FPU per core
    - 4 FLOPS/clk peak per core
  - Integrated Memory Controller
    - Up to 12.8 GB/s
    - DDR2-800 MHz or DDR2-667 MHz
- **Scalability**
  - 48-bit Physical Addressing
- **Compatibility**
  - Same power/thermal envelopes as 2nd / 3rd generation AMD Opteron™ CPU

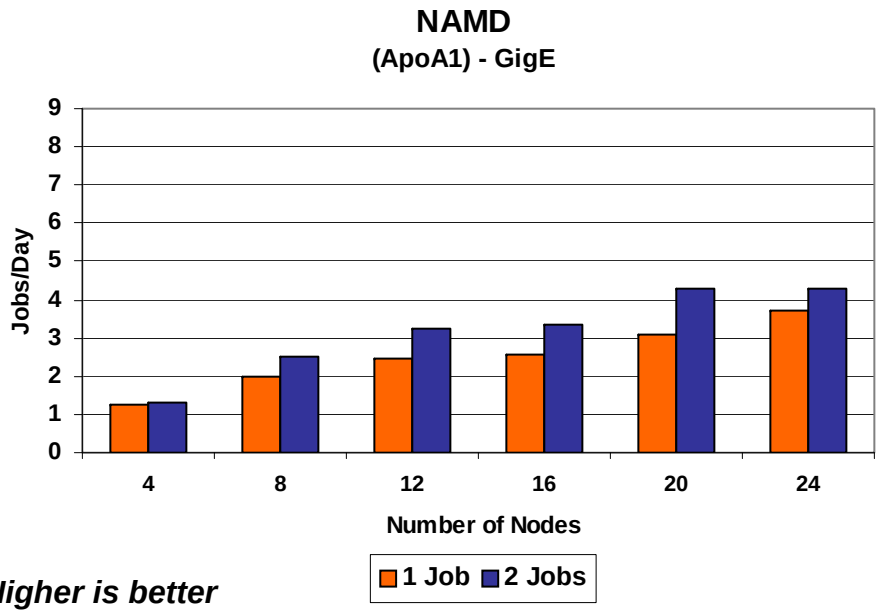


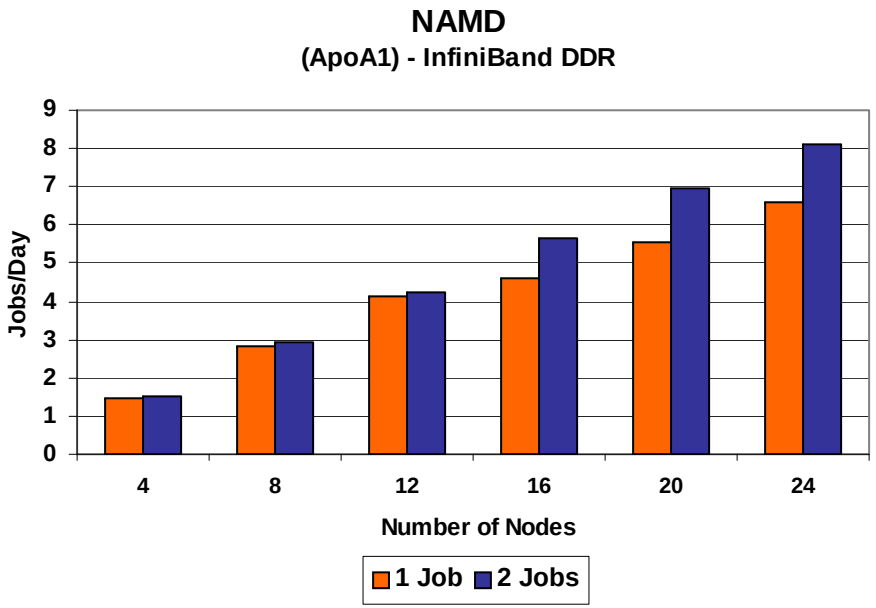
Dell PowerEdge Servers helping Simplify IT

- **System Structure and Sizing Guidelines**
  - 24-node cluster build with Dell PowerEdge™ SC 1435 Servers
  - Servers optimized for High Performance Computing environments
  - Building Block Foundations for best price/performance and performance/watt
- **Dell HPC Solutions**
  - Scalable Architectures for High Performance and Productivity
  - Dell's comprehensive HPC services help manage the lifecycle requirements.
  - Integrated, Tested and Validated Architectures
- **Workload Modeling**
  - Optimized System Size, Configuration and Workloads
  - Test-bed Benchmarks
  - ISV Applications Characterization
  - Best Practices & Usage Analysis

NAMD Benchmark Results – Productivity

- **Case 1: Dedicated hardware resource for NAMD**
- **Input Date: ApoA1**
  - Benchmark comprises 92K atoms of lipid, protein, and water
  - Models a bloodstream lipoprotein particle
  - One of the most used data sets for benchmarking NAMD
- **Increasing number of concurrent jobs increases cluster productivity**
- **InfiniBand enables higher performance and productivity**

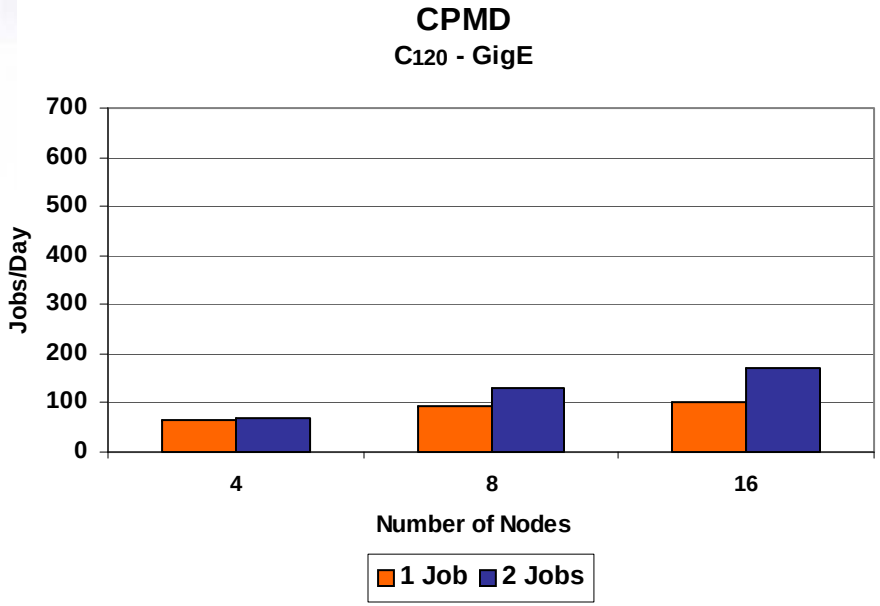


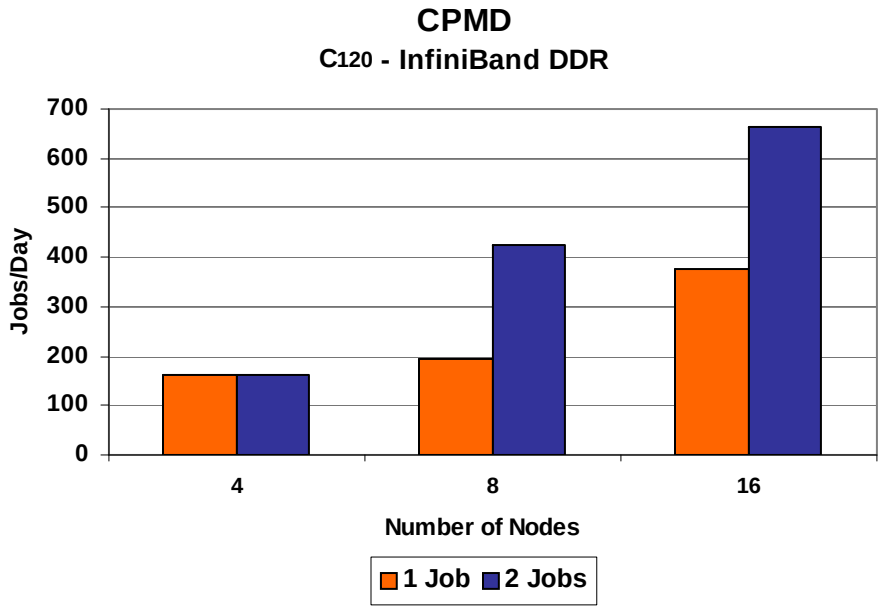


Higher is better

CPMD Benchmark Results – Productivity

- **Case 2: Dedicated hardware resource for CPMD**
- **Benchmark Data: C_{120} - 120 carbon atoms**
- **Running two jobs in parallel increases cluster productivity**
- **InfiniBand enables higher performance and scalability than GigE**





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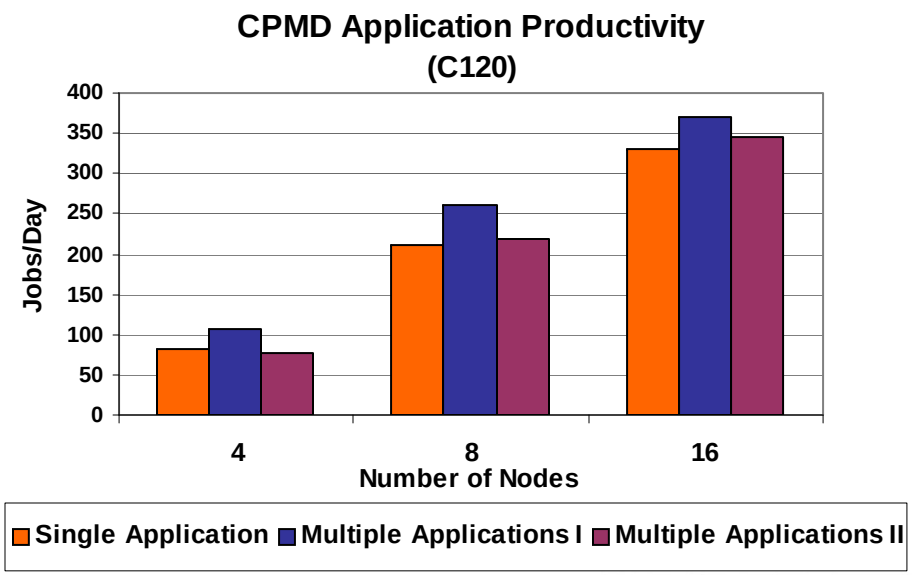
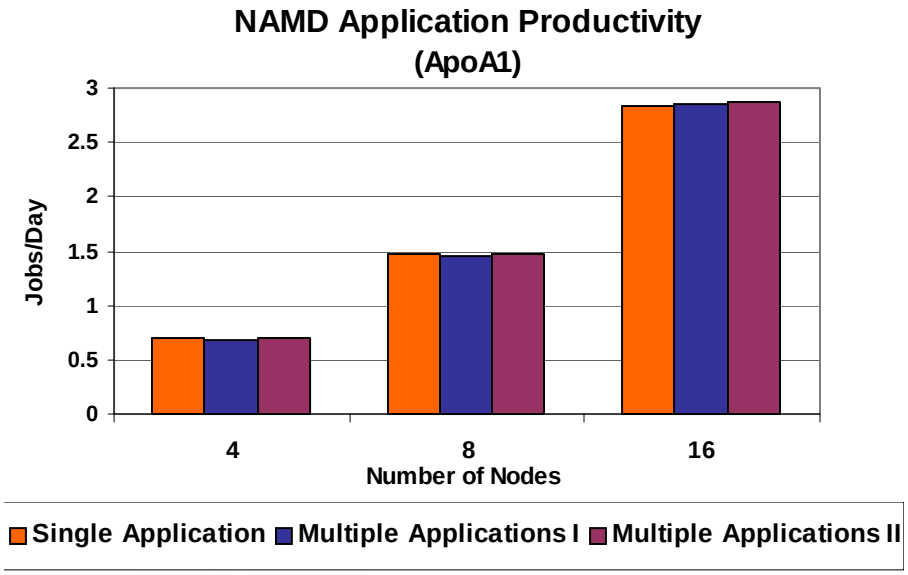
Multiple Applications – CPMD and NAMD

- **Case 3 – HPC as a Service (HPCaaS)**
- **HW platform to serve multiple applications at the same time**
  - CMPD and NAMD
- **Multiple test scenarios will be presented in the following slides**
  - Each describes different allocation methods of the HW system per service
    - Service refers to a single application
    - At least 2 applications will be served at a given time
  - Each scenario will be to compared to a dedicated HW per applications approach
    - Evaluation metric: productivity (number of jobs per day)

Multiple Applications – CPMD and NAMD

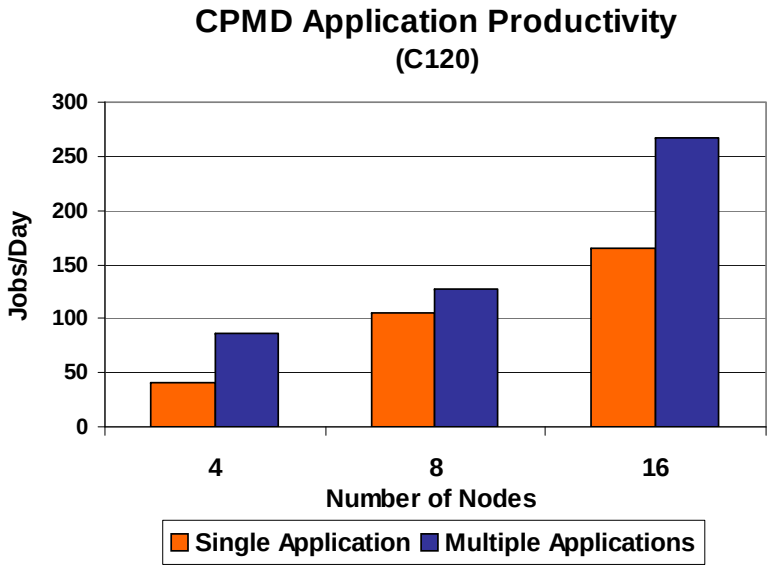
- **Test Scenario:**
  - Single Application approach:
    - Two NAMD jobs in parallel for half day then two CPMD jobs for the other half day
  - Multiple Applications approach
    - One CPMD job and one NAMD job simultaneously on the cluster for a full day
    - Case I:4 cores for each application (2 cores on each CPU)
    - Case II: One application per CPU socket
- **Running CPMD and NAMD in parallel improves CPMD productivity**
- **Distributing CPMD processes to two sockets has better performance**
  - Versus using an entire CPU (socket) per applications
- **NAMD shows negligible productivity difference under the three scenarios**

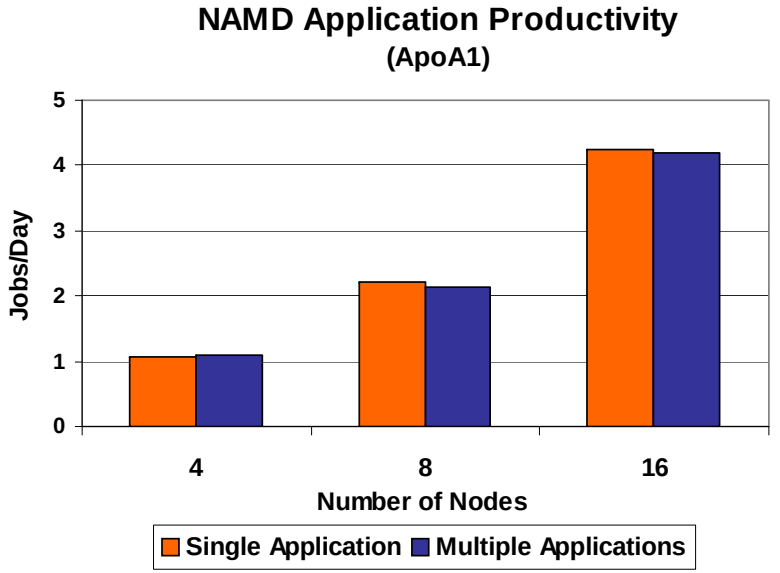




Multiple Applications – CPMD + NAMD

- **Test Scenario:**
  - Single Application
    - Two NAMD jobs in parallel for 3/4 day then two CPMD jobs for 1/4 day
  - Multiple Applications
    - One CPMD job and one NAMD job simultaneously on the cluster for a full day
    - 6 cores for NAMD (3 cores on each CPU), 2 cores for CPMD (1 core on each CPU)
- **Running CPMD and NAMD in parallel improves CPMD productivity by up to 61%**
- **NAMD shows negligible productivity difference under the two scenarios**





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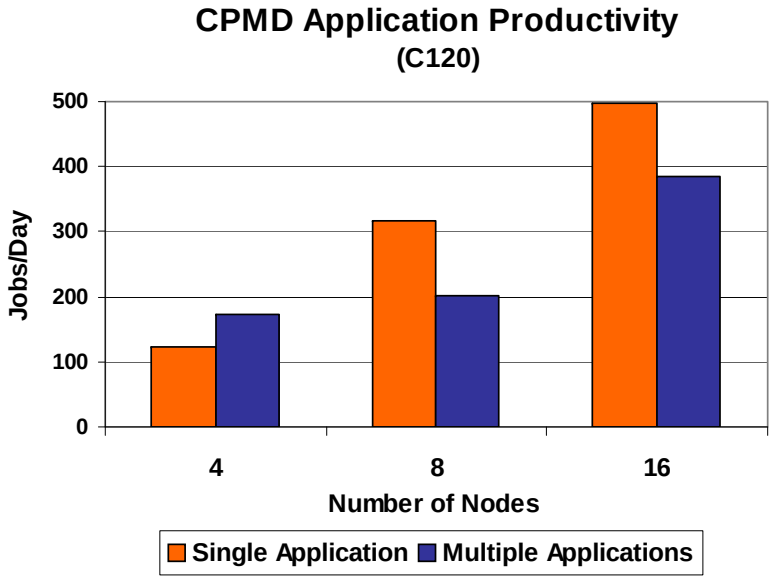
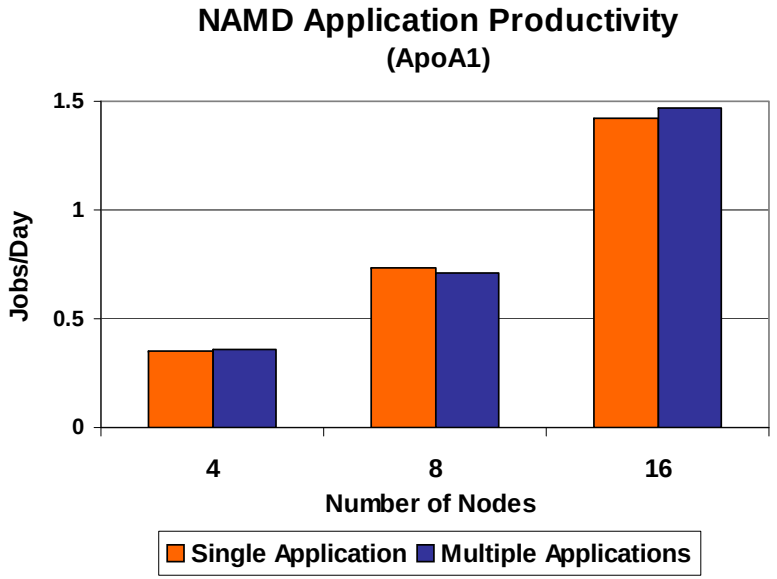
InfiniBand DDR

Multiple Applications – CPMD + NAMD

- **Test Scenario:**
  - Single Application
    - Two NAMD jobs in parallel for 1/4 day then two CPMD jobs for 3/4 day
  - Multiple Applications
    - One CPMD job and one NAMD job simultaneously on the cluster for a full day
    - 2 cores for NAMD (1 core on each CPU), 6 cores for CPMD (3 cores on each CPU)
- **Running CPMD with less cores decreases CPMD productivity**
- **NAMD shows negligible productivity difference under the two scenarios**





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InfiniBand DDR

Results Summary

- **NAMD**
  - Increase number of jobs running on the each node improves productivity
  - InfiniBand provides nearly doubled performance of GigE
  - GigE does not scale beyond 20 nodes
- **CPMD**
  - Higher productivity is gained with 2 parallel CPMD jobs on the cluster
  - InfiniBand delivers up to 300% higher productivity vs GigE
- **CPMD and NAMD simultaneously – HPC as a Service (HPCaaS)**
  - It is feasible and productive to run CPMD and NAMD simultaneously on a single system
  - When enough core were allocated, CPMD productivity was increased
  - NAMD demonstrates same level of productivity
  - NAMD consumes large portion of the systems resources
    - Having more than a single NAMD and CPMD jobs will not increase productivity

Conclusions

- **HPC as a Service enables greater systems flexibility**
  - Eliminates the need for dedicated HW resources per applications
  - Simplifies usage models
  - Enables dynamic allocation per given task
- **Effectively model needs to take into consideration**
  - Applications sensitivity points and applications bottlenecks
  - Minimum HW resource requirements per applications
  - Matching up applications with different hardware requirements
- **HPC as a Service for Bio-science applications (CMPD and NAMD)**
  - Enables increased or equal productivity versus dedicated HW resource
  - Method: allocation of 4 cores or less for CPMD, 4 cores or more for NAMD
    - Cores per application allocation – using both sockets demonstrate higher productivity
    - Better allocation of cores, memory and interconnect resources to minimize contention
    - NAMD requires more or equal compute resources than CPMD

Thank You

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