HPC2002 Result

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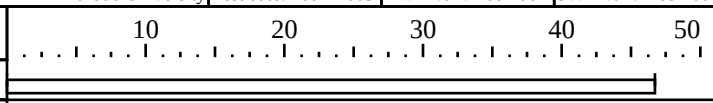
HP DL145

SPECchemM2002 = 46.7

SPEC license #: HPG0007A	Tested by: Purdue University	Test site: Purdue University	Test date: Jun-2005	HW Avail: Dec-2004	SW Avail: Dec-2004

Benchmark	Reference Time	Runtime	Ratio
371.gamess_m	86400	1849	46.7



Hardware

CPU:	AMD Opteron(tm) Processor 244
CPU MHz:	1800
FPU:	Integrated
CPU(s) enabled:	32 cores, 32 chips, 1 core/chip
CPU(s) orderable:	1 or 2 per node
Primary Cache:	64KB (I) micro-ops (trace) + 64KB (D) on chip
Secondary Cache:	1 MB on chip
L3 Cache:	N/A
Other Cache:	N/A
Memory:	4 GB DDR PC2700 CL2.5 ECC Registered per node
Disk Subsystem:	1x40 GB IDE (7200 RPM) per node
Other Hardware:	See File server and Network notes

Software

Parallel:	MPI
Processes-Threads:	32
MPI Processes:	32
OpenMP Threads:	--
Operating System:	RedHat Enterprise Linux, Advanced Server version 3 (4)
Compiler:	Intel(R) C++ Compiler for Intel(R) EM64T, Version 8.1 Build 20040812 Intel(R) Fortran Compiler for Intel(R) EM64T, Version 8.1 Build 20040812
File System:	NFS shared file system
System State:	Multi-user
Other Software:	mpich-vapi (see notes for configuration)

Notes/Tuning Information

```
Tested by Purdue University
Flags (Fortran & C):
CPP Flags: -E -traditional -DMPI -DSPEC_HPG_MPI_INT4
COPTIMIZE = -O2 -static -fp_port -DMPI -DSPEC_HPG_MPI_INT4 -DFORTRAN_UNDERSCORE
FOPTIMIZE = -O3 -static -i8 -fp_port -unroll
LDOPTIONS = -Vaxlib

Submit command to run MPI application:
PBS Version: PBSPro_5.4.2.43350
PBS Command to get resources (for cyclic allocation of processes):
qsub -I -q preempto -lnodes=16:ppn=2,walltime=1:00:00
use_submit_for_speed=1
submit=mpirun -np 32 -hostfile $PBS_NODEFILE $command
Cluster config:
Nodes and file server use NFS shared file system
Two chips per node
File server:
2 x 3.06 GHz Intel Xeon processors
4 GB DDR PC2100 CL2.5 ECC Registered Memory
5 x 72 GB 10K RPM SCSI Drives
Hardware RAID-5 (Dell PERC/3Di option)
Debian Linux, 3.1 "sarge"
ext3 local file system
NFS shared file system
Network (for computation and file server):
Topspin Infinihost HCA, 4x Infiniband
Switches:
Topspin ts270 aggregation switch
Topspin ts120 leaf switches

Environment variables set in .cshrc
setenv MPI_ENABLED ENABLED
setenv IRCDATA gamess_us.irc
setenv INPUT gamess_us.F05
setenv PUNCH gamess_us.dat
setenv INTGRLS gamess_us.F08
setenv AOINTS gamess_us.F08
setenv MOINTS gamess_us.F09
```

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Notes/Tuning Information (Continued)

```
setenv DICTNRY gamess_us.F10
setenv DRTFILE gamess_us.F11
setenv CIVECTR gamess_us.F12
setenv NTNFMLA gamess_us.F13
setenv CIINTS gamess_us.F14
setenv WORK15 gamess_us.F15
setenv WORK16 gamess_us.F16
setenv CSFSAVE gamess_us.F17
setenv FOCKDER gamess_us.F18
setenv DASORT gamess_us.F20
setenv JKFILE gamess_us.F23
setenv ORDINT gamess_us.F24
setenv EFPIND gamess_us.F25
MPICH-1.2.5 Configuration
CC=/opt/intel_cc_81/bin/icc
CXX=/opt/intel_cc_81/bin/icc
FC=/opt/intel_fc_81/bin/ifort
F90=/opt/intel_fc_81/bin/ifort
```