HPC2002 Result

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Dell PowerEdge 1750 cluster

SPECchemM2002 = 33.9

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

Benchmark	Reference Time	Runtime	Ratio
371.gamess_m	86400	2549	33.9

Hardware

CPU:	Intel Pentium4 Xeon
CPU MHz:	3060
FPU:	Integrated
CPU(s) enabled:	32 cores, 32 chips, 1 core/chip (Hyper-Threading Technology enabled)
CPU(s) orderable:	1 or 2 per node
Primary Cache:	12KB (I) micro-ops (trace) + 8KB (D) on chip
Secondary Cache:	512KB on chip
L3 Cache:	1 MB on chip
Other Cache:	N/A
Memory:	2 GB DDR PC2100 CL2.5 ECC Registered per node
Disk Subsystem:	1x36 GB SCSI 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 C++ Compiler- icc, Version 8.1 Build 20050309Z for Linux Intel Fortran Compiler- ifort, Version 8.1 Build 20050309Z for Linux
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: -I. -C -P -traditional -Dmpi -DSPEC_HPG_MPI_INT4
OPTIMIZE = -O3 -i8 -march=pentium4 -mcpu=pentium4 -axW -tpp7
LDOPTIONS = -O3

Submit command to run MPI application:
PBS Version: PBSPro 5.4.1.41640
PBS Command to get resources (for cyclic allocation of processes):
qsub -I -q preemptx -lnodes=16:IB:ppn=2,walltime=2:00:00
use_submit_for_speed=1
MPI_COMM_SIZE=32
submit=mpirun -np 32 $PBS_NODEFILE $command
Cluster config:
Nodes and file server use NFS shared file system
Two CPUs per node, Hyper-Threading Technology enabled
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):
Infiniband: Topspin HBAs, Topspin 120 switches

All BIOS parameters left with factory defaults.
For a description of Intel compiler flags,portability flags,
and system parameters used to generate this result,please refer
to PURDUE-20050329-INTEL-LINUX-XEON.txt in the flags directory
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
```

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Notes/Tuning Information (Continued)

```
setenv AOINTS gamess_us.F08
setenv MOINTS gamess_us.F09
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
./configure --with-device=ch_vapi --with-arch=LINUX --without-mpe
--without-romio --disable-sharedlib
```