



HPC2002 Result

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DELL
PowerEdge 1750 cluster

SPECchemM2002 = 33.2

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	2604	33.2

Hardware		Software	
CPU:	Intel Xeon processor	Parallel:	MPI
CPU MHz:	3060	Processes-Threads:	32
FPU:	Integrated	MPI Processes:	32
CPU(s) enabled:	32 cores, 32 chips, 1 core/chip (Hyper-Threading Technology enabled)	OpenMP Threads:	-
CPU(s) orderable:	1 or 2 per node	Operating System:	RedHat Enterprise Linux, Advanced Server version 3 (4)
Primary Cache:	12KB (I) micro-ops (trace) + 8KB (D) on chip	Compiler:	Intel C++ Compiler- icc, Version 8.1
Secondary Cache:	512KB on chip		Build 20050309Z for Linux
L3 Cache:	1 MB on chip		Intel Fortran Compiler- ifort, Version 8.1
Other Cache:	N/A		Build 20050309Z for Linux
Memory:	2 GB DDR PC2100 CL2.5 ECC Registered per node	File System:	NFS shared file system
Disk Subsystem:	1x36 GB SCSI per node	System State:	Multi-user
Other Hardware:	See File server and Network notes	Other Software:	MPICH-1.2.6 (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: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):

Cisco 6509 Gigabit Ethernet Switch

Built-in Gigabit Ethernet Adapters

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 INTGRSL gamess_us.F08

```



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Notes/Tuning Information (Continued)

```
setenv APOINTS 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-1.2.6 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_p4 --without-mpe --disable-sharedlib \
-rsh=/usr/bin/ssh
```