# HPC2002 Result

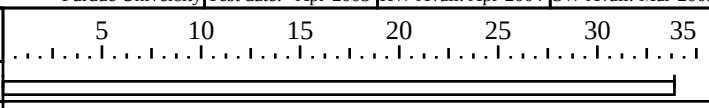


## Dell
## PowerEdge 1750 cluster

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<br>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 \
-cflags="-D_SMP_ -DUSE_STDARG  -DLAZY_MEM_UNREGISTER -DUSE_INLINE \
-DRDMA_FAST_PATH -DEARLY_SEND_COMPLETION -D_REENTRANT -O2  \
-DVIADEV_RPUT_SUPPORT -MD -fpic -DMT_LITTLE_ENDIAN  -D__LINUX__ \
-DVAPI -DTS_HOST_DRIVER -DCPU_X86 \
-I/usr/local/topspin/include -I/usr/local/topspin/include/vapi \
-L/usr/local/topspin/lib " \
-lib="-lvapi -lmtl_common -lmpga -lmosal -lpthread"
```