



# HPC2002 Result

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**DELL**  
**PowerEdge 1750 cluster**

**SPECchemM2002 = 41.1**

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	5	10	15	20	25	30	35	40	45
371.gamess_m	86400	2101	41.1									

### Hardware

CPU: Intel Xeon processor  
 CPU MHz: 3060  
 FPU: Integrated  
 CPU(s) enabled: 64 cores, 64 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: 64  
 MPI Processes: 64  
 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-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=32:ppn=2,walltime=1:00:00
```

```
use_submit_for_speed=1
```

```
MPI_COMM_SIZE=64
```

```
submit=mpirun -np 64 \${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 INTGRS 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/fort
F90=/opt/intel_fc_81/bin/fort
./configure --with-device=ch_p4 --without-mpe --disable-sharedlib \
-rsh=/usr/bin/ssh
```