



HPC2002 Result

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Dell
PowerEdge 1750 cluster

SPECchemM2002 = 43.0

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 | 2010 | 43.0 | | | | | | | | | |

Hardware

CPU: Intel Pentium4 Xeon
 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: None
 Memory: 2 GB DDR PC2100 CL2.5 ECC Registered per node
 Disk Subsystem: 1x36 GB SCSI per node
 Other Hardware: see 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-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=32:IB: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):

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 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 NTNFMFLA 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/fort
F90=/opt/intel_fc_81/bin/fort
./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"
```