



HPC2002 Result

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HP DL145

SPECchemM2002 = 60.1

SPEC license #: HPG0007A | Tested by: Purdue University | Test site: Purdue University | Test date: Jun-2005 | HW Avail: Dec-2004 | SW Avail: Dec-2004

Benchmark	Reference Time	Runtime	Ratio
371.gamess_m	86400	1438	60.1

Hardware		Software	
CPU:	AMD Opteron(tm) Processor 244	Parallel:	MPI
CPU MHz:	1800	Processes-Threads:	64
FPU:	Integrated	MPI Processes:	64
CPU(s) enabled:	64 cores, 64 chips, 1 core/chip	OpenMP Threads:	--
CPU(s) orderable:	1 or 2 per node	Operating System:	RedHat Enterprise Linux, Advanced Server version 3 (4)
Primary Cache:	64KB (I) micro-ops (trace) + 64KB (D) on chip	Compiler:	Intel(R) C++ Compiler for Intel(R) EM64T, Version 8.1 Build 20040812
Secondary Cache:	1 MB on chip		Intel(R) Fortran Compiler for Intel(R) EM64T, Version 8.1 Build 20040812
L3 Cache:	N/A	File System:	NFS shared file system
Other Cache:	N/A	System State:	Multi-user
Memory:	4 GB DDR PC2700 CL2.5 ECC Registered per node	Other Software:	mpich-vapi (see notes for configuration)
Disk Subsystem:	1x40 GB IDE (7200 RPM) per node		
Other Hardware:	See File server and Network notes		

Notes/Tuning Information

Tested by Purdue University

Flags (Fortran & C):

```

CPP Flags: -E -traditional -DMPI -DSPEC_HPG_MPI_INT4
OPTIMIZE = -O2 -static -fp_port -DMPI -DSPEC_HPG_MPI_INT4 -DFORTRAN_
FOPTIMIZE = -O3 -static -i8 -fp_port -unroll
LDOPTIONS = -Vaxlib

```

Submit command to run MPI application:

PBS Version: PBSPro_5.4.2.43350

PBS Command to get resources (for cyclic allocation of processes):

```

qsub -I -q preempto -lnodes=16:ppn=2,walltime=1:00:00
use_submit_for_speed=1
submit=mpirun -np 64 -hostfile \${PBS_NODEFILE} $command

```

Cluster config:

Nodes and file server use NFS shared file system

Two Chips per node

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):

Topspin Infinihost HCA, 4x Infiniband

Switches:

Topspin ts270 aggregation switch

Topspin ts120 leaf switches

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
setenv AOINTS gamess_us.F08
setenv MOINTS gamess_us.F09

```



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Notes/Tuning Information (Continued)

```
setenv DICTNRY gamess_us.F10
setenv DRTRFILE 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"
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-20050624-AMD-LINUX-OPTERON.txt in the flags directory
```