



HPC2002 Result

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Hewlett-Packard Company
HP Cluster Platform 4000 w/XC (DL145 G2)

SPECchemM2002 = **93.1**

SPEC license #: HPG0001 | Tested by: Hewlett-Packard Company | Test site: Houston, Texas | Test date: Aug-2005 | HW Avail: Jun-2005 | SW Avail: Oct-2005

Benchmark	Reference Time	Runtime	Ratio
371.gamess_m	86400	928	93.1

Hardware		Software	
CPU:	AMD Opteron(tm) Processor 252	Parallel:	MPI
CPU MHz:	2600	Processes-Threads:	96
FPU:	Integrated	MPI Processes:	96
CPU(s) enabled:	96 cores, 96 chips, 1 core/chip	OpenMP Threads:	--
CPU(s) orderable:	1 to 2 per node	Operating System:	XC Linux for High Performance Computing v3.0
Primary Cache:	64KBI + 64KBD (on chip) per core	Compiler:	Pathscale 2.2 Fortran Compiler Pathscale 2.2 C Compiler
Secondary Cache:	1 MB on chip	File System:	NFS Shared File System
L3 Cache:	--	System State:	Multi-user
Other Cache:	None	Other Software:	HP-MPI 2.1.1, LSF 6.1.7, SLURM 0.5.0-10
Memory:	4 GB DDR PC3200 per node (8x512K)		
Disk Subsystem:	1x80GB SATA disk (root)		
Other Hardware:	See below for a more complete system description		

Notes/Tuning Information

Peak Flags:

```
mpif90 -Ofast -I. -i8
FOPTIMIZE = -DSPEC_HPG_MPI_INT4 -DBITS64
```

```
mpicc -Ofast -I.
CPORTABILITY = -DLINUXIA64
COPTIMIZE = -DSPEC_HPG_MPI_INT4 -DBITS64
```

```
Preprocessing:
-I. -C -P -traditional
```

```
ENV_SPEC_HPG_PARALLEL=MPI
```

Flags file description HP-MPI-Pathscale-20050913.txt

Peak User Environment:

```
bsub -n 96 ./runspec -c linux_amd_psc --reportable chem_m
use_submit_for_speed=1
submit = \${MPI_ROOT}/bin/mpirun -srun
\${SPEC}/runenv taskset 0x3 $command < /dev/null
```

```
runenv defines the chem environment variables
-srun launches one process per processor
consisting of the command which follows.
taskset execs its arguments and bind proceses
to processors according to mask.
$command is generated by the SPEC tools.
```

System Description

HPC Cluster Platform is a Hewlett-Packard preconfigured and factory built hardware and software solution scalable from 5 to 512 nodes. The product used in these submissions is an HP Cluster Platform model 4000.

For Product Information see www.hp.com and search for
HPC Clusters Platforms
<http://www.hp.com/techservers/clusters/ucp/index.html>
XC Clusters



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Notes/Tuning Information (Continued)

http://www.hp.com/techservers/clusters/xc_clusters.html

For detailed quick specs, search www.hp.com and search for:

HP Cluster Platform 3000 and HP Cluster Platform 4000

http://h18000.www1.hp.com/products/quickspecs/12306_div/12306_div.HTML

XC System Software V2.1 quickspecs

http://h18000.www1.hp.com/products/quickspecs/12094_div/12094_div.HTML

Underlying Cluster compute nodes:

HP ProLiant DL145 G2 server

48 compute nodes used for this run.

Network (for computation)

Voltaire Infiniband HCA 400Ex

Voltaire leaf switches - ISR 9024 (1 per 12 nodes)

Voltaire aggregation switch - ISR 9288 (12 ports per leaf switch)

Network (for File Server)

ProCurve 2848 Gb Ethernet Switches (1 per 40 nodes)

File Server

HP ProLiant DL585

two AMD Opteron (tm) Processor 850 2400MHz

8 GB Memory 4 2GB PC2100 Dimms

146 GB SCSI 10000 Disk

runenv script to propogate environment

```
#!/bin/csh
```

```
setenv IRCDATA ./gamess_us.irc
```

```
setenv INPUT ./gamess_us.F05
```

```
setenv PUNCH ./gamess_us.dat
```

```
setenv INTGRLS ./gamess_us.F08
```

```
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 NTNFMILA ./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
```

```
setenv MPI_ENABLED ENABLED
```