HPC2002 Result

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Hewlett-Packard Company

HP Cluster Platform 4000 w/XC (DL145 G2)

SPECchemM2002 = 57.2

SPEC license #: HPG2116	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	1511	57.2

Hardware

CPU:	AMD Opteron(tm) Processor 252
CPU MHz:	2600
FPU:	Integrated
CPU(s) enabled:	24 cores, 24 chips, 1 core/chip
CPU(s) orderable:	1 to 2 per node
Primary Cache:	64KBI + 64KBD (on chip) per core
Secondary Cache:	1 MB on chip
L3 Cache:	--
Other Cache:	None
Memory:	4 GB DDR PC3200 per node (8x512K)
Disk Subsystem:	1x80GB SATA disk (root)
Other Hardware:	See below for a more complete system descrition

Software

Parallel:	MPI
Processes-Threads:	24
MPI Processes:	24
OpenMP Threads:	--
Operating System:	XC Linux for High Performance Computing v3.0
Compiler:	Pathscale 2.2 Fortran Compiler Pathscale 2.2 C Compiler
File System:	NFS Shared File System
System State:	Multi-user
Other Software:	HP-MPI 2.1.1, LSF 6.1.7, SLURM 0.5.0-10

Notes/Tuning Information

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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 24 ./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 procesor
        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)

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        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
  12 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 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
 setenv MPI_ENABLED ENABLED
```