

GAMESS-2012May01 for UV1000

Webpage

<http://www.msg.ameslab.gov/GAMESS/GAMESS.html>

Version

May 1, 2012

Tools for Compiling

▶ Intel Compiler 12.1.2.273

Necessary Files for Compiling

▶ gamess-2012May01.tar.gz (from GAMESS webpage)

▶ rungms.patch

Content of rungms.patch

```
--- rungms.orig 2012-08-15 14:07:02.535168674 +0900
+++ rungms 2012-08-15 14:10:11.368169006 +0900
@@ -57,9 +57,9 @@
# See also a very old LoadLeveler "ll-gms" for some IBM systems.
#
set TARGET=sockets
-set SCR=/scr/$USER
-set USERSCR=~$USER/scr
-set GMSPATH=/u1/mike/gamess
+set SCR=/work/users/$USER/scr.$$
+if (! -d $SCR) mkdir $SCR
+set GMSPATH=/local/apl/uv/gamess2012May01
#
set JOB=$1 # name of the input file xxx.inp, give only the xxx part
set Verno=$2 # revision number of the executable created by 'lkd' step
@@ -89,16 +89,11 @@
    uniq $TMPDIR/machines
endif
if ($SCHED == PBS) then
- set SCR=/scratch/$PBS_JOBID
+# set SCR=/scratch/$PBS_JOBID
    echo "PBS has assigned the following compute nodes to this run:"
    uniq $PBS_NODEFILE
endif
#
-echo "Available scratch disk space (Kbyte units) at beginning of the job is"
-df -k $SCR
-echo "GAMESS temporary binary files will be written to $SCR"
-echo "GAMESS supplementary output files will be written to $USERSCR"
-
# this added as experiment, February 2007
# its intent is to detect large arrays allocated off the stack
limit stacksize 8192
@@ -131,6 +126,15 @@
    endif
endif

+set dir=`dirname $JOB`
+set USERSCR=`cd $dir; pwd`
+
+echo "Available scratch disk space (Kbyte units) at beginning of the job is"
+df -k $SCR
+echo "GAMESS temporary binary files will be written to $SCR"
+echo "GAMESS supplementary output files will be written to $USERSCR"
+
+
# define many environment variables setting up file names.
# anything can be overridden by a user's own choice, read 2nd.
source $GMSPATH/gms-files.csh
@@ -255,53 +259,55 @@
# NODE= physical enclosure (box/blade)
#
# 1. Sequential execution is sure to be on this very same host
- if ($NCPUS == 1) then
+### if ($NCPUS == 1) then
```

```

+### set NNODES=1
+### set HOSTLIST=('hostname')
+### endif
+####
+#### 2. This is an example of how to run on a multi-core SMP enclosure,
+#### where all CPUs (aka COREs) are inside a -single- NODE.
+#### At other locations, you may wish to consider some of the examples
+#### that follow below, after commenting out this ISU specific part.
+### if ($NCPUS > 1) then
+### switch ('hostname')
+### case se.msg.chem.iastate.edu:
+### case sb.msg.chem.iastate.edu:
+###     if ($NCPUS > 2) set NCPUS=2
+###     set NNODES=1
+###     set HOSTLIST=('hostname':cpus=$NCPUS)
+###     breaksw
+### case br.msg.chem.iastate.edu:
+###     if ($NCPUS > 4) set NCPUS=4
+###     set NNODES=1
+###     set HOSTLIST=('hostname':cpus=$NCPUS)
+###     breaksw
+### case cd.msg.chem.iastate.edu:
+### case zn.msg.chem.iastate.edu:
+### case ni.msg.chem.iastate.edu:
+### case co.msg.chem.iastate.edu:
+### case pb.msg.chem.iastate.edu:
+### case bi.msg.chem.iastate.edu:
+### case po.msg.chem.iastate.edu:
+### case at.msg.chem.iastate.edu:
+### case sc.msg.chem.iastate.edu:
+###     if ($NCPUS > 4) set NCPUS=4
+###     set NNODES=1
+###     set HOSTLIST=('hostname':cpus=$NCPUS)
+###     breaksw
+### case ga.msg.chem.iastate.edu:
+### case ge.msg.chem.iastate.edu:
+### case gd.msg.chem.iastate.edu:
+###     if ($NCPUS > 6) set NCPUS=6
+###     set NNODES=1
+###     set HOSTLIST=('hostname':cpus=$NCPUS)
+###     breaksw
+### default:
+###     echo I do not know how to run this node in parallel.
+###     exit 20
+### endsw
+### endif
+### set NNODES=1
- set HOSTLIST=('hostname')
- endif
-#
-# 2. This is an example of how to run on a multi-core SMP enclosure,
-# where all CPUs (aka COREs) are inside a -single- NODE.
-# At other locations, you may wish to consider some of the examples
-# that follow below, after commenting out this ISU specific part.
- if ($NCPUS > 1) then
- switch ('hostname')
- case se.msg.chem.iastate.edu:
- case sb.msg.chem.iastate.edu:
-     if ($NCPUS > 2) set NCPUS=2
-     set NNODES=1
-     set HOSTLIST=('hostname':cpus=$NCPUS)
-     breaksw
- case br.msg.chem.iastate.edu:
-     if ($NCPUS > 4) set NCPUS=4
-     set NNODES=1
-     set HOSTLIST=('hostname':cpus=$NCPUS)
-     breaksw
- case cd.msg.chem.iastate.edu:
- case zn.msg.chem.iastate.edu:
- case ni.msg.chem.iastate.edu:
- case co.msg.chem.iastate.edu:
- case pb.msg.chem.iastate.edu:
- case bi.msg.chem.iastate.edu:
- case po.msg.chem.iastate.edu:
- case at.msg.chem.iastate.edu:
- case sc.msg.chem.iastate.edu:
-     if ($NCPUS > 4) set NCPUS=4

```

```

-     set NNODES=1
-     set HOSTLIST=(`hostname`:cpus=$NCPUS)
-     breaksw
-     case ga.msg.chem.iastate.edu:
-     case ge.msg.chem.iastate.edu:
-     case gd.msg.chem.iastate.edu:
-         if ($NCPUS > 6) set NCPUS=6
-         set NNODES=1
-         set HOSTLIST=(`hostname`:cpus=$NCPUS)
-         breaksw
-     default:
-         echo I do not know how to run this node in parallel.
-         exit 20
-     endsw
- endif
+ set HOSTLIST=(`hostname`:cpus=$NCPUS)
#
# 3. How to run in a single computer, namely the "localhost", so
# this computer needn't have a proper Internet name.
@@ -353,90 +359,90 @@
# names into the HOSTLIST string for the kickoff program,
# and to request the host name of the fast network adapters.
#
- if ($?PBS_JOBID) then
-#
-# The IBM cluster has two Gigabit adapters in each 4-way SMP,
-# while the AXP cluster is based on a Myrinet network.
- if (`uname` == AIX) set NETEXT=".gig.,gig2"
- if (`uname` == Linux) set NETEXT=".myri"
-#
-# repeated host names in the PBS host file indicate being assigned
-# CPUs in the same SMP enclosure, which we must count up correctly.
-# Fortunately PBS gives duplicate host names in a row, not scrambled.
-# The number of hosts in the PBS node file (nmax) should equal the
-# requested processor count, NCPUS. We need to count duplicates
-# in order to learn the number of SMP enclosures, NNODES, and how
-# many CPUs inside each SMP were assigned (NSMPCPU). For example,
-# if we are assigned the host names "a a a b b c c c" we must build
-# the string "a:cpus=3 b:cpus=2 c:cpus=3" so that ddikick.x will
-# know the SMP structure of the assigned node names. (C-shell handles
-# variable substitution followed by colon gracefully by ${HOST}:cpus.)
-#
- set HOSTLIST=()
- set nmax=`wc -l $PBS_NODEFILE`
- set nmax=${nmax}[1]
- if ($nmax != $NCPUS) then
-     echo There is processor count confusion
-     exit
- endif
-#     1st host in the list is sure to be a new SMP enclosure
- set MYNODE=`sed -n -e "1 p" $PBS_NODEFILE`
- set MYNODE=`echo $MYNODE | awk '{split($0,a,"."); print a[1]}'`
-#     IPROC counts assigned processors (up to NCPUS),
-#     NNODES counts number of SMP enclosures.
-#     NSMPCPU counts processors in the current SMP enclosure
- @ IPROC = 2
- @ NNODES = 1
- @ NSMPCPU = 1
- set spacer1=":cpus="
- set spacer2=":netext="
- while($IPROC <= $nmax)
-     set MYPROC=`sed -n -e "$IPROC p" $PBS_NODEFILE`
-     set MYPROC=`echo $MYPROC | awk '{split($0,a,"."); print a[1]}'`
-     if($MYPROC != $MYNODE) then
-         set HOSTLIST = ($HOSTLIST $MYNODE$spacer1$NSMPCPU$spacer2$NETEXT)
-         set MYNODE=$MYPROC
-         @ NSMPCPU = 0
-         @ NNODES++
-     endif
-     @ IPROC++
-     @ NSMPCPU++
- end
- set HOSTLIST = ($HOSTLIST $MYNODE$spacer1$NSMPCPU$spacer2$NETEXT)
- endif
-#
-# we have now finished setting up a correct HOSTLIST.
-# uncomment the next two if you are doing script debugging.

```

```

-#--echo "The generated host list is"
-#--echo $HOSTLIST
-#
-#
-#   choose remote shell execution program.
-#   Parallel run do initial launch of GAMESS on remote nodes by the
-#   following program. Note that the authentication keys for ssh
-#   must have been set up correctly.
-#   If you wish, choose 'rsh' using .rhosts authentication on next line.
-   setenv DDI_RSH ssh
-#
-   if($DDI_RSH == ssh) then
-       setenv DDI_RCP scp
-   else
-       setenv DDI_RCP rcp
-   endif
-
-#   One way to be sure that the master node of each subgroup
-#   has its necessary copy of the input file is to stuff a
-#   copy of the input file onto every single node right here.
-   if ($GDDIjob == true) then
-       @ n=2 # master in master group already did 'cp' above
-       while ($n <= $NNODES)
-           set host=$HOSTLIST[$n]
-           set host=`echo $host | cut -f 1 -d :` # drop anything behind a colon
-           echo $DDI_RCP $SCR/$JOB.F05 ${host}:$SCR/$JOB.F05
-           $DDI_RCP $SCR/$JOB.F05 ${host}:$SCR/$JOB.F05
-           @ n++
-       end
-   endif
+###   if ($?PBS_JOBID) then
+####
+#####   The IBM cluster has two Gigabit adapters in each 4-way SMP,
+#####   while the AXP cluster is based on a Myrinet network.
+###   if (`uname` == AIX) set NETEXT=".gig.gig2"
+###   if (`uname` == Linux) set NETEXT=".myri"
+####
+#####   repeated host names in the PBS host file indicate being assigned
+#####   CPUs in the same SMP enclosure, which we must count up correctly.
+#####   Fortunately PBS gives duplicate host names in a row, not scrambled.
+#####   The number of hosts in the PBS node file (nmax) should equal the
+#####   requested processor count, NCPUS. We need to count duplicates
+#####   in order to learn the number of SMP enclosures, NNODES, and how
+#####   many CPUs inside each SMP were assigned (NSMPCPU). For example,
+#####   if we are assigned the host names "a a a b b c c c" we must build
+#####   the string "a:cpus=3 b:cpus=2 c:cpus=3" so that ddickick.x will
+#####   know the SMP structure of the assigned node names. (C-shell handles
+#####   variable substitution followed by colon gracefully by ${HOST}:cpus.)
+####
+###   set HOSTLIST=()
+###   set nmax=`wc -l $PBS_NODEFILE`
+###   set nmax=$nmax[1]
+###   if ($nmax != $NCPUS) then
+###       echo There is processor count confusion
+###       exit
+###   endif
+#####   1st host in the list is sure to be a new SMP enclosure
+###   set MYNODE=`sed -n -e "1 p" $PBS_NODEFILE`
+###   set MYNODE=`echo $MYNODE | awk '{split($0,a,"."); print a[1]}'`
+#####   IPROC counts assigned processors (up to NCPUS),
+#####   NNODES counts number of SMP enclosures.
+#####   NSMPCPU counts processors in the current SMP enclosure
+###   @ IPROC = 2
+###   @ NNODES = 1
+###   @ NSMPCPU = 1
+###   set spacer1=":cpus="
+###   set spacer2=":netext="
+###   while($IPROC <= $nmax)
+###       set MYPROC=`sed -n -e "$IPROC p" $PBS_NODEFILE`
+###       set MYPROC=`echo $MYPROC | awk '{split($0,a,"."); print a[1]}'`
+###       if($MYPROC != $MYNODE) then
+###           set HOSTLIST = ($HOSTLIST $MYNODE$spacer1$NSMPCPU$spacer2$NETEXT)
+###           set MYNODE=$MYPROC
+###           @ NSMPCPU = 0
+###           @ NNODES++
+###       endif
+###   @ IPROC++

```

```

##### @ NSMPCPU++
##### end
##### set HOSTLIST = ($HOSTLIST $MYNODE$spacer1$NSMPCPU$spacer2$NETEXT)
##### endif
#####
##### we have now finished setting up a correct HOSTLIST.
##### uncomment the next two if you are doing script debugging.
#####--echo "The generated host list is"
#####--echo $HOSTLIST
#####
#####
##### choose remote shell execution program.
##### Parallel run do initial launch of GAMESS on remote nodes by the
##### following program. Note that the authentication keys for ssh
##### must have been set up correctly.
##### If you wish, choose 'rsh' using .rhosts authentication on next line.
##### setenv DDI_RSH ssh
#####
##### if($DDI_RSH == ssh) then
##### setenv DDI_RCP scp
##### else
##### setenv DDI_RCP rcp
##### endif
#####
##### One way to be sure that the master node of each subgroup
##### has its necessary copy of the input file is to stuff a
##### copy of the input file onto every single node right here.
##### if ($GDDIjob == true) then
##### @ n=2 # master in master group already did 'cp' above
##### while ($n <= $NNODES)
##### set host=$HOSTLIST[$n]
##### set host=`echo $host | cut -f 1 -d ':'` # drop anything behind a colon
##### echo $DDI_RCP $SCR/$JOB.F05 ${host}:$SCR/$JOB.F05
##### $DDI_RCP $SCR/$JOB.F05 ${host}:$SCR/$JOB.F05
##### @ n++
##### end
##### endif

#
# Just make sure we have the binaries, before we try to run
@@@ -455,9 +461,10 @@@
#
if ($DDI_VER == new) then
set echo
- $GMSPATH/ddikick.x $GMSPATH/gamesess.$VERNO.x $JOB \
- -ddi $NNODES $NCPUS $HOSTLIST \
- -scr $SCR < /dev/null
##### $GMSPATH/ddikick.x $GMSPATH/gamesess.$VERNO.x $JOB \
##### -ddi $NNODES $NCPUS $HOSTLIST \
##### -scr $SCR < /dev/null
+ $GMSPATH/ddikick.x dplace -s1 $GMSPATH/gamesess.$VERNO.x $JOB -ddi $NNODES $NCPUS ${HOSTLIST} -scr $SCR < /dev/null
unset echo
else
set path=($GMSPATH $path)
@@@ -1051,13 +1058,13 @@@
if (-e $SCR/$JOB.molf) mv $SCR/$JOB.molf $USERSCR
if (-e $SCR/$JOB.mkl) mv $SCR/$JOB.mkl $USERSCR
if (-e $SCR/$JOB.xyz) mv $SCR/$JOB.xyz $USERSCR
-ls $SCR/${JOB}*.cube > $SCR/${JOB}.lis
+(ls $SCR/${JOB}*.cube > $SCR/${JOB}.lis) >& /dev/null
if (! -z $SCR/${JOB}.lis) mv $SCR/${JOB}*.cube $USERSCR
rm -f $SCR/${JOB}.lis
-ls $SCR/${JOB}*.grd > $SCR/${JOB}.lis
+(ls $SCR/${JOB}*.grd > $SCR/${JOB}.lis) >& /dev/null
if (! -z $SCR/${JOB}.lis) mv $SCR/${JOB}*.grd $USERSCR
rm -f $SCR/${JOB}.lis
-ls $SCR/${JOB}*.csv > $SCR/${JOB}.lis
+(ls $SCR/${JOB}*.csv > $SCR/${JOB}.lis) >& /dev/null
if (! -z $SCR/${JOB}.lis) mv $SCR/${JOB}*.csv $USERSCR
rm -f $SCR/${JOB}.lis
#

```

Procedure of Compiling

```

#!/bin/csh -f
umask 022
set file_gameess=/home/users/${USER}/build/gamesess2012May01/gamesess-2012May01.tar.gz

```

```

set work=/work/users/${USER}
set gamess=gamess2012May01
set patch_rungms=/home/users/${USER}/build/gamess2012May01/ccuv/rungms.patch
#-----
cd ${work}
if (-d ${gamess}) then
  mv ${gamess} ${gamess}-erase
  rm -rf ${gamess}-erase &
endif
#-----
tar xzf ${file_gamess}
mv gamess ${gamess}
cd ${work}/${gamess}
expect <<EXPECT
spawn ./config
expect "After the new window is open"
send "\r"
expect "please enter your target machine name:"
send "linux64\r"
expect "GAMESS directory?"
send "\r"
expect "GAMESS build directory?"
send "\r"
expect "Version?"
send "\r"
expect "Please enter your choice of FORTRAN:"
send "ifort\r"
expect "Version?"
send "12\r"
expect "hit <return> to continue after digesting this message."
send "\r"
expect "hit <return> to continue to the math library setup."
send "\r"
expect "Enter your choice of 'mkl' or 'atlas' or 'acml' or 'none':"
send "mkl\r"
expect "MKL pathname?"
send "/opt/intel/mkl\r"
expect "MKL version (or 'skip')?"
send "10.2.5.035\r"
expect "please hit <return> to compile the GAMESS source code activator"
send "\r"
expect "please hit <return> to set up your network for Linux clusters."
send "\r"
expect "communication library ('sockets' or 'mpi')?"
send "sockets\r"
expect eof
EXPECT
#-----
cd ${work}/${gamess}/ddi
sed -e 's/MAXCPUS = 16/MAXCPUS = 1024/' -e 's/MAXNODES = 256/MAXNODES = 2/' compddi > compddi1024
csh ./compddi1024 >& compddi.log
mv ddikick.x ../
cd ${work}/${gamess}
./compall >& compall.log
./lked >& lked.log
#-----
chmod -R o-rwx source object
find . -name "src" | xargs chmod -R o-rwx
#-----
patch -p0 < ${patch_rungms}

```
