

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"
```

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+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 ddickick.x will
-# know the SMP structure of the assigned node names. (C-shell handles
-# variable substitution followed by colon gracefully by ${HOST}:cpus.)

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-#
- 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
- 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"
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#####
##### 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 ddick.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.
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```

```

#####
#### 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 $GMSPATH/games.$VERNO.x $JOB \
-   -ddi $NNODES $NCPUS $HOSTLIST \
-   -scr $SCR < /dev/null
+### $GMSPATH/ddikick.x $GMSPATH/games.$VERNO.x $JOB \
+### -ddi $NNODES $NCPUS $HOSTLIST \
+### -scr $SCR < /dev/null
+   $GMSPATH/ddikick.x dplace -s1 $GMSPATH/games.$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_gamess=/home/users/${USER}/build/games2012May01/games-2012May01.tar.gz
set work=/work/users/${USER}
set gamess=games2012May01
set patch_rungms=/home/users/${USER}/build/games2012May01/ccuv/rungms.patch
#-----
cd ${work}

```

```

if (-d ${gameess}) then
  mv ${gameess} ${gameess}-erase
  rm -rf ${gameess}-erase &
endif
#-----
tar xzf ${file_gameess}
mv gameess ${gameess}
cd ${work}/${gameess}
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 ${work}/${gameess}/ddi
sed -e 's/MAXCPUS = 16/MAXCPUS = 1024/' -e 's/MAXNODES = 256/MAXNODES = 2/' compddi > compddi1024
csh ./compddi1024 >& compddi.log
mv ddikick.x ../
cd ${work}/${gameess}
./compall >& compall.log
./lked >& lked.log
#-----
chmod -R o-rwx source object
find . -name "src" | xargs chmod -R o-rwx
#-----
patch -p0 < ${patch_rungms}

```