

GAMESS-2012May01 for UV2000

ウェブページ

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

バージョン

May 1, 2012

ビルド環境

- Intel Compiler 12.1.2.273

ビルドに必要なファイル

- gamess-2012May01.tar.gz (GAMESSのウェブページからダウンロードしたもの)
- rungms.patch

rungms.patchの内容

```
--- 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 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.)

```

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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

```

```

- 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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+#### CPUs in the same SMP enclosure, which we must count up correctly.
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+#### 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($0,a,"."); print a[1]}`
+#### IPROC counts assigned processors (up to NCPUS),
+#### NNODES counts number of SMP enclosures.
+#### NSMPCPU counts processors in the current SMP enclosure
+#### @ IPROC = 2
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+#### @ NSMPCPU = 1
+#### set spacer1=":cpus="
+#### set spacer2=":netext="
+#### while($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"
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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 $GMSPATH/gamess.$VERNO.x $JOB \
-   -ddi $NNODES $NCPUS $HOSTLIST \
-   -scr $SCR < /dev/null
+### $GMSPATH/ddikick.x $GMSPATH/gamess.$VERNO.x $JOB \
+### -ddi $NNODES $NCPUS $HOSTLIST \
+### -scr $SCR < /dev/null
+   $GMSPATH/ddikick.x dplace -s1 $GMSPATH/gamess.$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
#

```

ビルド手順

```

#!/bin/csh -f
umask 022
set file_gamess=/home/users/${USER}/build/gamess2012May01/gamess-2012May01.tar.gz
set work=/work/users/${USER}
set gamess=gamess2012May01
set patch_rungms=/home/users/${USER}/build/gamess2012May01/ccuv/rungms.patch
#-----
cd ${work}

```

```

if (-d ${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}

```