I have been trying to compile nwchem with openmpi for several days with no success. I'm using fedora 15 and the following script to compile nwchem 6.0 but I don't know if it is working.

Script code

[code][wcucluster.master@wcucluster ~]$ cat buildit
#!/bin/tcsh
echo "let's build NWCHEM"
setenv LARGE_FILES TRUE
setenv LIB_DEFINES -DDFLT_TOT_MEM=16777216
setenv TCGRSH /usr/bin/ssh
setenv NWCHEM_TOP /home/wcucluster.master/nwchem-6.0
cd $NWCHEM_TOP/src
setenv NWCHEM_TARGET LINUX
setenv NWCHEM_TARGET_CPU SGITFP
setenv USE_MPI y
setenv USE_MPIF y
setenv MPI_LOC /usr/lib/openmpi
setenv MPI_LIB $MPI_LOC/lib
setenv MPI_INCLUDE $MPI_LOC/include
setenv LIBMPI "-L $MPI_LIB -lmpi -lopen-pal -lopen-rte -lmpi_f90 -lmpi_f77"
cd $NWCHEM_TOP/src/util
cd $NWCHEM_TOP/src
make nwchem_config NWCHEM_MODULES=all[/code]

Resulting terminal output

[code][wcucluster.master@wcucluster ~]$ ./buildit
let's build NWCHEM
make -C config -f make_nwchem_config NWCHEM_MODULES="all"
echo \# This configuration generated automatically on \
    `hostname` at `date` > nwchem_config.h
echo "# Request modules from user: all" >> nwchem_config.h
echo "NW_MODULE_SUBDIRS = NWints atomscf ddscf gradients moints nwdft rimp2 stepper driver optim cphf ccsd vib mcscf prepar esp hessian selci dplot mp2_grad qhop property nwpw fft argos analyz nwmd cafe space drdy vscf qmmm qmd etrans tce bq cons perfm dntmc dangchang ccca" >> nwchem_config.h
echo "NW_MODULE_LIBS = -lccsd -lmcscf -lselci -lmp2 -lmoints -lstepper -ldriver -loptim -lnwdft -lgradients -lcphf -lesp -lddscf -ldangchang -lguess -lhessian -lvib -lnwcutil -lrimp2 -lproperty -lnwints -largos -lprepar -lnwmd -lnwpw -lofpw -lpaw -lpspw -lband -lnwpwlib -lcafe -lspace -lanalyze -lqhop -lpfft -ldplot -ldrdy -lvscf -lqmmm -lqmd -letrans -lpspw -ltce -lbq -lcons -lperfm -ldntmc -lccca" >> nwchem_config.h
echo "EXCLUDED_SUBDIRS = develop scfaux plane_wave oimp2 rimp2_grad python diana uccsdt geninterface transport smd nbo leps" >> nwchem_config.h
echo "CONFIG_LIBS = " >> nwchem_config.h
echo \# This configuration generated automatically on \
    `hostname` at `date` > NWCHEM_CONFIG

```
echo "# Request modules from user: all" >> NWCHEM_CONFIG
echo The following subdirectories are built: >> NWCHEM_CONFIG
echo NWints analyz argos atomscf bq cafe ccca ccsd cons cphf dangchang ddscf dntmc dplot drdy driver
esp etrans fft gradients hessian mcscf moints mp2_grad nwdft nwmd nwpw optim perfm prepar
property qhop qmd qmmm rimp2 selci space stepper symmetry tce vib vscf >> NWCHEM_CONFIG
echo corresponding to these libraries: >> NWCHEM_CONFIG
echo -lnwints -lanalyze -largos -lguess -lbq -lcafe -lccca -lccsd -lcons -lcphf -ldangchang -lddscf -ldntmc -
ldplot -ldrdy -ldriver -lesp -letrans -lpfft -lgradients -lhessian -lmcscf -lmoints -lmp2 -lnwdft -lnwmd -
lnwpw -lofpw -lpaw -lpspw -lband -lnwpwlib -loptim -lperfm -lprepar -lproperty -lqhop -lqmd -lqmmm -
lrimp2 -lselci -lspace -lstepper -lnwcutil -ltce -lvib -lvscf >> NWCHEM_CONFIG
echo >> NWCHEM_CONFIG
echo The following directories are excluded from the build: >> NWCHEM_CONFIG
echo develop scfaux plane_wave oimp2 rimp2_grad python diana uccsdt geninterface transport smd
nbo leps >> NWCHEM_CONFIG
echo and these routines will be replaced by stubs: >> NWCHEM_CONFIG
echo crossing debtest dia_input diana gasdev geninterface jantest jvltest jvltest2 kgdtest leps_energy
leps_gradient mc_data mc_driver mc_init mc_main md_data md_driver md_set moints_screen
mymc_input mymd_input nbo_input oimp2 player plnwv plnwv_input python_input raktest rimp2g
rjhtest smd_input task_nbo task_python task_smd task_smd_dynamics task_smd_energy transp_input
transport uccsdt uccsdtest urand  >> NWCHEM_CONFIG
echo "No extra configuration libraries were added " >> NWCHEM_CONFIG
cp census.skeleton ../stubs.F
for routine in crossing debtest dia_input diana gasdev geninterface jantest jvltest jvltest2 kgdtest
leps_energy leps_gradient mc_data mc_driver mc_init mc_main md_data md_driver md_set
moints_screen mymc_input mymd_input nbo_input oimp2 player plnwv plnwv_input python_input
raktest rimp2g rjhtest smd_input task_nbo task_python task_smd task_smd_dynamics
task_smd_energy transp_input transport uccsdt uccsdtest urand; do \
  sed s/STUBROUTINE/$routine/g stub.skeleton >> ../stubs.F ; \
done
[wcucluster.master@wcucluster ~]$[/code]
```

The operation completes very quickly which makes me believe it was not successful. When I modify the script to this I receive terminal output with errors.

Script code

```
[code][wcucluster.master@wcucluster ~]$ cat buildit
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setenv LARGE_FILES TRUE
setenv LIB_DEFINES -DDFLT_TOT_MEM=16777216
setenv TCGRSH /usr/bin/ssh
setenv NWCHEM_TOP /home/wcucluster.master/nwchem-6.0
cd $NWCHEM_TOP/src
setenv NWCHEM_TARGET LINUX
setenv NWCHEM_TARGET_CPU SGITFP
setenv USE_MPI y
setenv USE_MPIF y
```

setenv MPI_LOC /usr/lib/openmpi
setenv MPI_LIB $MPI_LOC/lib
setenv MPI_INCLUDE $MPI_LOC/include
setenv LIBMPI "-L $MPI_LIB -lmpi -lopen-pal -lopen-rte -lmpi_f90 -lmpi_f77"
cd $NWCHEM_TOP/src/util
make version
make
cd $NWCHEM_TOP/src
make link[/code]

Resulting terminal output

[code][wcucluster.master@wcucluster ~]$ ./buildit
let's build NWCHEM
./catsrc nwchem.F config tools include basis geom inp input pstat rtdb task symmetry util peigs perfm bq cons blas lapack NWints atomscf ddscf gradients moints nwdft rimp2 stepper driver optim cphf ccsd vib mcscf prepar esp hessian selci dplot mp2_grad qhop property nwpw fft argos analyz nwmd cafe space drdy vscf qmmm qmd etrans tce bq cons perfm dntmc dangchang ccca | \
awk -f ids.awk > util_version.F
-rw-r-----. 1 wcucluster.master wcucluster.master 1609700 Oct 21 18:59 util_version.F
/home/wcucluster.master/nwchem-6.0/bin/LINUX_SGITFP/depend.x -I/home/wcucluster.master/nwchem-6.0/src/tools/include > dependencies
f77 -c -fno-second-underscore -fno-f90 -ffixed-line-length-72 -ffixed-form -malign-double -fno-globals -Wno-globals -fno-silent -g output.f
output:
doutput:
ioutput:
make: *** No rule to make target `/home/wcucluster.master/nwchem-6.0/src/include/mafdecls.fh', needed by `/home/wcucluster.master/nwchem-6.0/lib/LINUX_SGITFP/libnwcutil.a(errquit.o)'. Stop.
make nwchem.o stubs.o
f77 -fno-second-underscore -fno-f90 -ffixed-line-length-72 -ffixed-form -malign-double -fno-globals -Wno-globals -fno-silent -g -I. -I/home/wcucluster.master/nwchem-6.0/src/include -I/home/wcucluster.master/nwchem-6.0/src/tools/include -DLINUX -DPARALLEL_DIAG -DCOMPILATION_DATE="'`date +%a_%b_%d_%H:%M:%S_%Y`'" -DCOMPILATION_DIR="'/home/wcucluster.master/nwchem-6.0'" -DNWCHEM_BRANCH="'6.0'" -c -o nwchem.o nwchem.F
nwchem.F:4: mafdecls.fh: No such file or directory
nwchem.F:5: global.fh: No such file or directory
nwchem.F:6: rtdb.fh: No such file or directory
nwchem.F:7: tcgmsg.fh: No such file or directory
nwchem.F:8: pstat.fh: No such file or directory
nwchem.F:10: inp.fh: No such file or directory
make[1]: *** [nwchem.o] Error 1
make: *** [link] Error 2
[wcucluster.master@wcucluster ~]$[/code]

The output pauses at "awk -f ids.awk > util_version.F" for a moment then continues with the resulting errors. Again I'm not sure if the compile is function properly. I'm compiling for openmpi using the package "openmpi.i686 installed using yum and "compat-gcc-34-g77.i686" also installed using yum with gnu make 3.82. I am fairly new to linux so any help would be appreciated.