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#####
#
# Makefile for UKRmol-in codes
#
# Possible invocations:
# make [with optional arguments]
# make clean
# (removes .o and .mod files)
# make cleanall
# (removes .o, .mod and executables)
#
# This Makefile DOES NOT NEED to be edited for use on different
# machines and/or with different compilers, etc.
# Default definitions of system-specific variables (the compiler,
# compiler flags, linear algebra libraries) can be found below.
# These settings can be overridden via command-line arguments to
# "make", or by setting the relevant variables appropriately in a
# file "make.inc" (copy, paste and edit the lines below that you
# want to change)
#
#####

#####
# Default settings for the system-dependent variables
# COMP=./home/singh/intel/composerxe/bin/ifort -w -mkl=sequential
# LINK=./home/singh/intel/composerxe/bin/ifort -static -mkl=sequential
COMP=ifort -w -mkl=sequential
LINK=ifort -static -mkl=sequential

OPT=-O3
NOOPT=-O0
OPT2=-O
# The following libraries should be included:
# Lapack and blas here:
LIB=./lib/liblapack.a
# Arpack here (compiled with sequential mkl):
LIBAR=./lib/libarpack_intel.a
#####

# The following include line must come after the system-specific defaults are set
# The leading "-" means that make will continue if the named file cannot be found
# (i.e. we wish to keep all the default settings)
-include make.inc

BINDIR = ./bin
SHELL = /bin/sh

TARGS = swscf swtrmo sword swedmos congen swmol3 swfjk gausprop gaustail psn scatci
denprop numcbas gtobas

.SUFFIXES:
.SUFFIXES: .f .f90 .o

```

all: \$(TARGS)

#.PHONY : all clean cleanall

clean:

rm -f \*.o \*.mod

cleanall:

rm -f \*.o \*.mod  
- cd ./bin && rm -f \$(TARGS)

%.o : %.f

\$(COMP) \$(OPT) -c \$<

# Make the local bin directory (note the -p option means that nothing is done if the dir already exists)

# in case it has accidentally been removed (etc.)

mkdir -p \$(BINDIR)

%.o : %.f90

\$(COMP) \$(OPT) -c \$<

# Make the local bin directory (note the -p option means that nothing is done if the dir already exists)

# in case it has accidentally been removed (etc.)

mkdir -p \$(BINDIR)

# special rule for swscf.f as optimisation breaks it

swscf.o: swscf.f

\$(COMP) \$(NOOPT) -c \$^

swscf: swscf.o swscf\_intPacking.o

\$(LINK) \$^ \$(LIB) -o \$@

mv -f swscf \$(BINDIR)

# special rule for swtrmo.f as errors occur with different optimisations

swtrmo.o: swtrmo.f

\$(COMP) \$(OPT2) -c \$^

swtrmo: swtrmo.o

\$(LINK) \$^ \$(LIB) -o \$@

mv -f swtrmo \$(BINDIR)

sword: sword.o

\$(LINK) \$^ -o \$@

mv -f sword \$(BINDIR)

swedmos: swedmos.o

\$(LINK) \$^ \$(LIB) -o \$@

mv -f swedmos \$(BINDIR)

congen: congen.o

\$(LINK) \$^ -o \$@

mv -f congen \$(BINDIR)

swmol3: swmol3.o  
\$(LINK) \$^ \$(LIB) -o \$@  
mv -f swmol3 \$(BINDIR)

swfjk: swfjk.o swfjk\_intPacking.o  
\$(LINK) \$^ -o \$@  
mv -f swfjk \$(BINDIR)

gausprop: gausprop.o  
\$(LINK) \$^ -o \$@  
mv -f gausprop \$(BINDIR)

gaustail: gaustail.o  
\$(LINK) \$^ -o \$@  
mv -f gaustail \$(BINDIR)

psn: psn.o  
\$(LINK) \$^ \$(LIB) -o \$@  
mv -f psn \$(BINDIR)

scatci: scatci.o davidson.o scatci\_intPacking.o  
\$(LINK) \$^ \$(LIB) \$(LIBAR) -o \$@  
mv -f scatci \$(BINDIR)

denprop: denprop.o denprop\_intPacking.o  
\$(LINK) \$^ \$(LIB) -o \$@  
mv -f denprop \$(BINDIR)

numcbas: numcbas.o  
\$(LINK) \$^ -o \$@  
mv -f numcbas \$(BINDIR)

gtobas: gtobas.o  
\$(LINK) \$^ -o \$@  
mv -f gtobas \$(BINDIR)