From: Robert Lucchese <lucchese@mail.chem.tamu.edu>
Subject: ckohn codes
Date: December 21, 2012 4:11:16 PM PST
To: smiyabe@stanford.edu

Dr. Miyabe:

The modified version of the complex kohn codes are in my dropbox account

https://www.dropbox.com/s/40c4stpp4frc3bd/ckohn.new.21.12.2012c.tgz

In the main directory there is a bash script (Makemesa.sh) that compiles all of the mesa and ckohn programs (except for hkohn). It just runs all of the make files in the various sub directories. You can use recent gfortran versions that have the -fdefault-integer-8 flag. To use larger basis sets the programs must be compiled using 8 byte integers. The Makemesa.sh uses various environment variables that tell the make files which compiler, which options and what BLAS library to use. The script gets these definitions from a file in the subdirectory ./include where there are a number of examples for different environments. Makemesa.sh assumes that the environment variable MACH has been defined. Then when you run

./Makemesa.sh all .gfi8

makes libraries and all programs using the gfortran compiler with 8 byte integers. The script will use the file include/$MACH.gfi8.sh to define the appropriate variables. The period in front of the compiler name is important to the script since that is how it identifies it as being a compiler name rather than a directory with source code. The script can also be used to compile just the libraries or one program

./Makemesa.sh clean (deletes all previously create executable files and libraries)
./Makemesa.sh lib .gfi8 (makes the libraries for the gfortran compiler with 8 byte integers)
./Makemesa.sh one m930 .gfi8 (makes the m930 program using the gfortran compiler with 8 byte integers)

The different machines that I have used have the following values of MACH

appleAbsoft11 - Mac OS X machines
intelmkl - intel Linux with ifort version 10
intelmklb - intel Linux with ifort version 12

the different compilers are

.f77i4 - 4 byte integers using the Absoft fortran compilers
.f77i8 - 8 byte integers using the Absoft fortran compilers
.g77 - 4 byte integers using the g77 compiler
.gfi4 - 4 byte integers using gfortran
.gfi8 - 8 byte integers using gfortran
.i4 - 4 byte integers using the intel ifort compiler
.i8 - 8 byte integers using the intel ifort compiler

You will also notice that in the include files there is a MAXCOR variable which is the size of blank common in terms of the number of integer words. Finally, some of the routines use the BLAS library. It is prudent to compile the BLAS library with the same compiler and options (e.g. the 8 byte integer option) as is used to compile the programs. Once you have done this you put the location of the BLAS library in the include file.

Let me know if you have any questions or problems getting this to work for you.

Sincerely,

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