MN-NWCHEMFM:
Minnesota NWCHEM Functional Module
Incorporating the M06 Suite of Functionals in the *NWCHEM* Program

Manual

Version 2.0

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Date of code completion: Jan. 2, 2007
Date of most recent change in this manual: Jan. 4, 2007

Contents

Executive summary

MN-NWCHEMFM, version 2.0 (Minnesota Gaussian Solvation Module, version 2.0) is a module for incorporation of the VS98, M06-L, M06-HF, M06, and M06-2X functionals into the *NWCHEM* code.

Code Distribution

NWCHEM is developed and distributed by Pacific Northwest National Laboratory, P. O. Box 999, Richland, Washington 99352 USA, and funded by the U. S. Department of Energy. Modified code may not be redistributed except by PNNL. The MN-NWCHEMFM package is prepared for transmitting code to the *NWCHEM* developers for release in an upcoming version of NWCHEM, for local use by the *MN-NWCHEMFM* developers and for trusted colleagues who have an urgent need for this code prior to the *NWCHEM* release.

Literature references for new functionals

VS98 (also called VSXC)

Voorhis, T. V.; Scuseria, G. E. *J. Chem. Phys.* **2006**, *125*, 194101.

M06-L

Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *125*, 194101.

M06-HF

Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2006**, *110*, 13126.

M06 and M06-2X

Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.,* submitted.

Usage

MN-NWCHEMFM allows users to perform calculations with the VS98 correlation functional and the M06 suite of functionals developed in the Truhlar group. The keywords for invoking these calculations are described here.

Required Keywords

vs98   This keyword specifies the VS98 (also called VSXC) functional.

m06-L   This keyword specifies the M06-L functional.

m06-hf   This keyword specifies the M06-HF functional.

m06   This keyword specifies the M06 functional.

m06-2x   This keyword specifies the M06-2X functional.

xvs98   This keyword specifies the GGA exchange part of the VS98 functional.

xm06-L   This keyword specifies the GGA exchange part of the M06-L functional.

xm06-hf   This keyword specifies the GGA exchange part of the M06-HF functional.

xm06   This keyword specifies the GGA exchange part of the M06 functional.

xm06-2x   This keyword specifies the GGA exchange part of the M06-2X functional.

cm06-L   This keyword specifies the meta-GGA correlation part of the M06-L functional.

cm06-hf   This keyword specifies the meta-GGA correlation part of the M06-HF functional.

cm06   This keyword specifies the meta-GGA correlation part of the M06 functional.

cm06-2x   This keyword specifies the meta-GGA correlation part of the M06-2X functional.

Package

The source code for the *MN-NWCHEMFM* was prepared at the University of Minnesota. It consists of a single directory, MNNWCHEMFM2.0, in which the implemented and modified subroutines necessary to run *MN-NWCHEMFM* reside.

Installing *MN-NWCHEMFM*

The *MN-NWCHEMFM* code is distributed as a compressed tar file named *MN-NWCHEMFM2.0.tar.gz*. It contains the necessary subroutines to run *MN-NWCHEMFM* with *NWCHEM*.
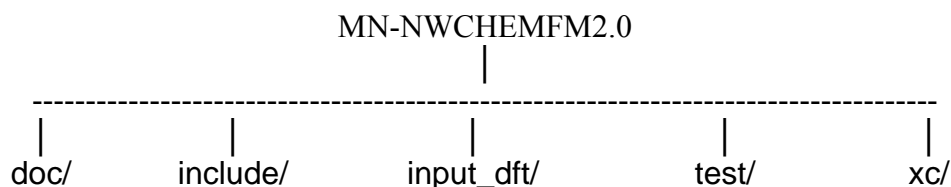
To uncompress, enter

```
gunzip  MN-NWCHEMFM2.0.tar.gz
```

The uncompressed file will be named `MN-NWCHEMFM2.0.tar` After extracting the files from the tar file, which can be done with the command:

```
tar -xvf MN-NWCHEMFM2.0.tar
```

a new directory, MN-NWCHEMFM2.0, is created. This directory contains all the files included in the distribution package, as follows

```
                        MN-NWCHEMFM2.0
                              |
       ---------------------------------------------------------------------------------
       |              |              |                     |              |
     doc/         include/       input_dft/             test/           xc/
```

doc: one file: MNNWFM2.0.UsersManual.pdf

input_dft: two files: dft_rdinput.F and xc_inp.F

test: ten files: test1.nw … test5.nw, test1.out, …, test5.out

xc   nine files: GNUmakefile, xc_chkgrad.F, xc_cm06.F, xc_xvs98.F,
               xc_xm06.F, xc_chktau.F, xc_eval_fnl.F

The following steps need to be taken to properly install *MN-NWCHEMFM*:

1) Make sure that the officially distributed NWCHEM-5.0 is properly installed.

2) Set the environment variable, NWCHEM_TOP, to the top directory of the NWCHEM tree, e.g.

```
setenv NWCHEM_TOP /homes/r30/zhaoy/nwchem-5.0
```

3) Go to the MN-NWCHEMFM2.0 directory. Issue the following command:

```
cp  -rf  input_dft/* $NWCHEM_TOP/src/nwdft/input_dft/
cp  -rf  xc/* $NWCHEM_TOP/src/nwdft/xc/
```

4) Following the standard procedure in the NWCHEM manual, recompile the NWCHEM code.

Platforms

MN-NWCHEMFM version 2.0 has been tested on the following platforms:

- IBM pSeries 690 and pSeries 655 Nodes (Power 4 processors) running AIX version 5.2 and compiled with the XL Fortran compiler version 9.1

- SGI Altix 3700 running the Linux operating system and compiled with the Intel Fortran compiler version 8.1

- IBM Blade285 running the Linux operating system and compiled with the PathScale(TM) EKOPath™ Compiler Suite: Version 2.5

Test Runs

Test run 1: VS98 single-point calculation of singlet H_2O with the 6-31+G(d) basis

Test run 2: M06-L single-point calculation calculation of closed-shell singlet Cu_2 with the LanL2DZ ECP basis set.

Test run 3: Unrestricted M06-HF force calculation of CH_3 with the 6-31+G(d) basis set.

Test run 4: M06 geometry optimization of HF with the 6-31+G(d) basis set.

Test run 5: Unrestricted M06-2X single-point energy calculation on NH2 + CH3 triplet transition state with 6-31+G(d) basis set.

Revision history and version summaries

MN-NWCHEMFM-v.1.0
Date: Feb. 21, 2006
Authors: Y. Zhao and D. G. Truhlar

This was the first version of *MN-NWCHEMFM*, and all functionals in this module, in particular, B1B95, BB1K, MPW1B95, MPWB1K, PW6B95, PWB6K, M05, and M05-2X, were subsequently incorporated in NWCHEM-v.5.0.

MN-NWCHEMFM-v2.0
Date: Jan. 4, 2007
Authors: Y. Zhao and D. G. Truhlar

The VS98, M06-L, M06-HF, M06, and M06-2X functionals have been implemented. This version was tested with NWCHEM-v.5.0.

Further information

If and when needed, updated information will be made available at the University of Minnesota Computational Chemistry Web site: http://comp.chem.umn.edu/MN-NWCHEMFM.

Acknowledgments