MANUAL

MN-VFM, version 2019-A:

Minnesota *VASP* Functional Module

Incorporating the MN12-L, N12, N12-SX, SOGGA, SOGGA11, SOGGA11-X, GAM, MN15-L, HLE17, revM06-L, and M06-SX functionals into the *VASP* program

Kaining Duanmu,[†,a] Sijie Luo,[†] Xiao He,[†,‡,ǂ,c] and Donald G. Truhlar[†,c]

[†]Department of Chemistry, Chemical Theory Center, and Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN 55455-0431, USA

[‡]Shanghai Engineering Research Center of Molecular Therapeutics and New Drug Development, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai, 200062, China

[ǂ]NYU–ECNU Center for Computational Chemistry at NYU Shanghai, Shanghai, 200062, China

[a] Email: duanmukn@gmail.com

[b] Email: xiaohe@phy.ecnu.edu.cn

[c] Email: truhlar@umn.edu

Date of final code modification: September 5, 2019

Date of most recent manual modification: September 7, 2019

Contents

1. Revision history

Version 1.0

Authors: Sijie Luo and Donald G. Truhlar

The functionals MN12-L, N12, N12-SX, SOGGA, SOGGA11, SOGGA11-X were added in *VASP*, the code was made compatible with *VASP* 5.3.2.

Version 2.0

Authors: Kaining Duanmu, Sijie Luo, and Donald G. Truhlar

The functional GAM was added in *VASP*, the code was made compatible with *VASP* 5.3.5.

Version 2.1

Authors: Kaining Duanmu, Sijie Luo, and Donald G. Truhlar

The functional MN15-L was added in *VASP*.

Version 2017

Authors: Kaining Duanmu, Sijie Luo, Pragya Verma, Xiao He, and Donald G. Truhlar

The functionals HLE17 and revM06-L were added in *VASP*.

Version 2017-A

Authors: Kaining Duanmu, Sijie Luo, Pragya Verma, Xiao He, and Donald G. Truhlar

We added two new test runs to the test suite.

Version 2019

Authors: Kaining Duanmu, Sijie Luo, Xiao He, and Donald G. Truhlar

The code was made compatible with *VASP* 5.4.4.

Version 2019-A

Authors: Kaining Duanmu, Sijie Luo, Xiao He, and Donald G. Truhlar

The functional M06-SX was added in the code cmpatible with *VASP* 5.4.4.

2. Installation

MN-VFM is a locally modified version of *VASP*. Our license does not permit the distribution of *VASP* code; the user should purchase the license of *VASP* separately.

The *MN-VFM* installation package is downloaded as one .tar compressed file. Untar the package (tar –xvf) and then make sure the following files and folders are present:

xclib.F xclib_grad.F metagga.F
MN-VFM_2019-A_Manual.pdf examples

Copy and replace the .F files in the vasp.5.4 directory, then compile *VASP*. If you have already compiled *VASP* correctly before with your own Makefile, then no modification in the Makefile is needed. If you are not able to compile *VASP*, please read the *VASP* manual and forum to obtain the correct Makefile before you compile the *MN-VFM* package.

The .pdf file in the distribution is the manual, and the examples folder contains 11 test runs including the input and output files.

3. Keywords for functionals

SOGGA
GGA = SA

SOGGA11
GGA = S1

SOGGA11-X
GGA = SX
LHFCALC = .TRUE.
AEXX = 0.401

N12
GGA = N2

N12-SX
GGA = NX
LHFCALC = .TRUE.
LHFSCREEN = 0.2

MN12-L

METAGGA = MN12L

GAM
GGA= GA

MN15-L
METAGGA = MN15L

HLE17
METAGGA = HLE17

revM06-L
METAGGA = revM06L

M06-SX
METAGGA = M06SX
LHFCALC = .TRUE.
HFSCREEN = 0.189
AEXX=0.335

4. Citation and references

If this code is used for published work, one should cite the reference(s) for the functional(s) used, and one should cite *MN-VFM*. The references are given in this section.

SOGGA

Zhao, Y.; Truhlar, D. G. Construction of a Generalized Gradient Approximation by Restoring the Density-Gradient Expansion and Enforcing a Tight Lieb-Oxford Bound. *J. Chem. Phys.* **2008**, *128*, 184109. dx.doi.org/10.1063/1.2912068

SOGGA11

Peverati, R.; Zhao, Y.; Truhlar, D. G. Generalized Gradient Approximation that Recovers the Second-Order Density-Gradient Expansion with Optimized Across-the-Board Performance. *J. Phys. Chem. Lett.* **2011**, *2*, 1991–1997. dx.doi.org/10.1021/jz200616w

SOGGA11-X

Peverati, R.; Truhlar, D. G. Communication: A Global Hybrid Generalized Gradient Approximation to the Exchange-Correlation Functional that Satisfies the Second-Order Density-Gradient Constraint and Has Broad Applicability in Chemistry. *J. Chem. Phys.* **2011**, *135*, 191102. dx.doi.org//10.1063/1.3663871

N12

Peverati, R.; Truhlar, D. G. Exchange–Correlation Functional with Good Accuracy for Both Structural and Energetic Properties While Depending Only on the Density and its Gradient. *J. Chem. Theory. Comput.* **2012**, *8*, 2310–2319. dx.doi.org/10.1021/ct3002656

N12-SX

Peverati, R.; Truhlar, D. G. Screened-Exchange Density Functionals with Broad Accuracy for Chemistry and Solid-State Physics. *Phys. Chem. Chem. Phys.* **2012**, *14*, 16187–16191. dx.doi.org/10.1039/C2CP42576A

MN12-L

Peverati, R.; Truhlar, D. G. An Improved and Broadly Accurate Local Approximation to the Exchange-Correlation Density Functional: The MN12-L Functional for Electronic Structure Calculations in Chemistry and Physics. *Phys. Chem. Chem. Phys.* **2012**, *14*, 13171–13174. dx.doi.org/10.1039/c2cp42025b

GAM

Yu, H. S.; Zhang, W.; Verma, P; He, X.; Truhlar, D. G. Nonseparable Exchange–Correlation Functional for Molecules, Including Homogeneous Catalysis Involving Transition Metals. *Phys. Chem. Chem. Phys.* **2015**, *17*, 12146–12160. dx.doi.org/10.1039/C5CP01425E

MN15-L

Yu, H. S.; He, X.; Truhlar, D. G. MN15-L: A New Local Exchange-Correlation Functional for Kohn–Sham Density Functional Theory with Broad Accuracy for Atoms, Molecules, and Solids *J. Chem. Theory. Comput.* **2016**, *12*, 1280–1293. dx.doi.org/10.1021/acs.jctc.5b01082

HLE17

Verma, P.; Truhlar, D. G. HLE17: An Improved Local Exchange–Correlation Functional for Computing Semiconductor Band Gaps and Molecular Excitation Energies. *J. Phys. Chem. C*, **2017**, *121*, 7144–7154.

revM06-L

Wang, Y.; Jin, X.; Yu, H. S.; Truhlar, D. G.; He, X. Revised M06-L Functional for Improved Accuracy on Chemical Reaction Barrier Heights, Noncovalent Interactions, and Solid-state Physics. *Proc. Natl. Acad. Sci. U.S.A.*, **2017**, *114*, 8487.

M06-SX

Wang, Y.; Verma, P.; Zhang, L.; Li, Y.; Liu, Z.; Truhlar, D. G.; He, X. M06-SX Screened-Exchange Density Functional for Chemistry and Solid-State Physics, submitted for publication.

MN-VFM – version 2019-A

Duanmu, K.; Luo, S.; He, X.; Truhlar, D. G. *MN-VFM* – version 2019-A, University of Minnesota: Minneapolis, 2019. https://comp.chem.umn.edu/mn-vfm/

5. Convergence issues

1. The global hybrid functional SOGGA11-X and screened hybrid functional N12-SX are much more time-consuming than their local counterparts. Always use ALGO = A or D for reliable SCF convergences. Please read the *VASP* manual for further information.

2. Meta functionals such as MN12-L, MN15-L, HLE17 revM06-L, and M06-SX (and M06-L, which is contained in the standard *VASP* program starting from version 5.2) require a two-step calculation for SCF convergence. (1) ALWAYS run a PBE calculation first. (2) Then follow with an M06-L, MN12-L, MN15-L, HLE17, revM06-L, or M06-SX calculation by reading in the PBE wave function, and use ALGO = A or D. In our experience, the SCF cycles may not converge appropriately if one does not folow this two-step procedurw.

6. PAW potentials

Meta functionals require the kinetic energy densities in the PAW potentials, and this is not done in the versions of PAW potentials that came with VASP 5.2 or earlier. If you are still using those old PAW potentials, MAKE SURE to download the latest ones from the *VASP* website. Otherwise unexpected errors or completely wrong results will be obtained for meta functionals.

7. VASP compatibility

MN-VFM version 2019-A has been developed and tested with *VASP* 5.4.4.

8. Further information

All the latest updates will be found at http://comp.chem.umn.edu/mn-vfm, please consult this Web page or the authors for further information.

9. Examples

There are 11 examples including the input and output files, in examples folder.

Example 1: O_2 molecule relaxation (geometry optimization) with GAM.

Example 2: CO molecule relaxation with MN15-L.

Example 3: Ni (FCC structure) lattice constant calculation with GAM.

Example 4: Ag (FCC structure) lattice constant calculation with MN15-L.

Example 5: Antiferromagnetic NiO calculation with GAM.

Example 6: Ni(100) surface relaxation with GAM.

Example 7: Cu(111) surface relaxation with MN15-L.

Example 8: O radical calculation with N12-SX.

Example 9: SiC relaxation with HLE17.

Example 10: S_2 molecule single-point calculation with revM06-L.

Example 11: S_2 molecule single-point calculation with M06-SX.