Release Note

July 18, 2017

Dear all,

We are pleased to announce that XMVB is now updated to Version 3.0. The stand-alone program is now ready for distribution, and the module for GAMESS-US will be prepared in the near future.

1 What's New in XMVB 3.0?

Following algorithms and techniques are implemented into XMVB 3.0 to enhance the capability:

1. Integrals, especially ERIs, can be computed directly in XMVB calculations now, instead of reading ERIs from file prepared with a third program. This may accelerate the computations when large number of basis functions are involved.

2. Cholesky decomposition (CD) of ERIs is supported by XMVB 3.0 which may accelerate VB calculations a lot when there are many inactive orbitals involved. Now VBSCF calculations can be carried out for more than one thousand basis functions.

3. Tensor-based formalism for valence bond theory is implemented in XMVB 3.0, which accelerates VBSCF calculations with larger active space.

4. State average VBSCF (SA-VBSCF) computations can be done now with XMVB by a simple keyword.

2 Installation Requirements

XMVB 3.0 currently supports Linux and Mac OS X. RHEL 6 is the recommended Linux distribution and any distribution with newer kernel is OK. The

version of Mac OS X should be at least 10.9. A valid Fortran compiler is essential to run XMVB jobs. For GNU Fortran compiler (gfortran), the version should be at least 4.4, which is the default in RHEL 6. For INTEL Fortran compiler (ifort), version at least 13 is strongly recommended since there are some bugs in ifort 12 which makes XMVB crash weirdly.

3 How to Get It?

If you are already a registered XMVB user, you may send email directly to Dr. Fuming Ying (email:fmying@xmu.edu.cn) to get the latest XMVB binary package. If you are interested in XMVB and want to be a user, please visit our official site (http://www.xmvb.org) to download the license agreement, sign and send it to Prof. Wei Wu (email:weiwu@xmu.edu.cn).