Small utility programs

There are several utility programs that you can find in the VB2000/TOOLS directory or the gamess/vb2000/SRC directory. They are generally self documenting. Open the program and read the header. In no particular order they are:-

1. getvbtime.f – If run in the directory where all the GAMESS test outputs are present, it will give the individual times and the total time for all tests.

2. getvbsotime.f – Does the same thing for the stand-alone version tests, but you have to create a list of the jobs first.

3. compare.f – This allows you to calculate the overlap between different VB orbitals for the same molecule, same basis set and same geometry but different methods. It allows to, for example, to explore the relationship of CASVB and SC orbitals. It requires the *.ovl file generated by $PRINTS, and $VEC blocks created by $VECONLY for each run. See the header of the program for more details.

4. get_gen_sto6g.f – This allows a variety of specialist STO-6G basis sets to be defined. This can include having separate exponents for s and p, optimal exponents, etc.

5. get-gms-bas.f – This reads a VB2000 basis set and converts it to the GAMESS format. It was used to get D95 which has been widely used in VB2000 stand-alone but is not defined in GAMESS.

6. get_cube_diff.f – This reads two CUBE files, evaluates the largest element in each and creates a file of the differences. It is used when the two files are the density of a VB function and the density of the GAMESS HF function created by the $DENSCUBE directive in GAMESS/VB2000.

7. molden2gmsvb.f – This reads a Molden file and creates a GAMESS/VB2000 input file that needs further editing, but it contains the basis set and geometry along with a $VEC group with the HF orbital from Molden. It also contains the HF orbital energies (eigenvalues), which other similar scripts do not.

8. xmvb_to_vec.f – This is a small Fortran program that creates a GAMESS(US) $VEC file of valence bond orbitals from a XMVB *.orb file. This has several uses:-
a) Along with the GAMESS *.log file, this *.vec file has be used by MacMolPlt to display the orbitals.
b) The *.vec file can be used by VB2000 as initial guess orbitals.

9. vbhelp - This is VB2000 help utility, modelled on gmshelp the GAMESS Unix on-line help - written by Greg Atchity, 25 March 1993. It requires VB-help-file, which is in the DOC directory,

molden2aim

If you are using Molden files, you are strongly advised to find molden2aim, written by W. Zou. See https://github.com/zorkzou/Molden2AIM/blob/master/README.md. It may be freely used and distributed under the MIT License. It comes as molden2aim.tar.gz. Open it up and you get a directory called m2a. This contains 4 directories:-

src – contains source file you can compile.
examples – contains 4 directories each of which contains a molden file. There are created by Cfour, Orca, Columbus and Molpro. They give a good example of the variation of molden files created by different programs.
util – contains a program, ReOrdAtm.f90, which reorders the atoms and does some clean up. I think this might be the program that is called reorderedf.F in readme.html linked from the mail readme file link above. It seems to be needed in some cases.
win – if you insist, this does what it suggests. It contains molden2aim.exe.

molden2aim is primarily designed to create *.wfn files for QTAIM work, but it also cleans up a Molden file. It removes non-standard blocks, but adds a Title block. It converts files created from a spherical harmonic basis set to one for cartesian basis sets. It is a most useful utility. If you move m2a-unix.ini from the src directory to your working directory and rename it as m2a.ini, it gives you more information when you run the program. For example, you may have to add a line such as "[Program] Orca" to the Molden file.

Stand-alone VB2000.

A Perl script, vbqa.pl, can be used to check the test set for the stand-alone program only. By default the output files are in the TEMPOUT directory, but a different directory can now (from July 2018) be given as a parameter to the ./vbqs.pl call.

Checkvbso does a ftnchk run on the stand-alone program. Ignore the mass of errors in vb2000ints.src. This needs to be replaced not improved. The variable set in vb2000-so.src but not used are variables that are read from external files but not needed. The other errors are post-fortran 77 constructs.