Description of utility-programs for DBSR complex (folder UTILS/DBSR_utils)

In addition to the main DBSR programs which were described separately, a number of short utility programs are available that assist in the processing and managing the data. Below is their short description with examples for those utilities which directly deal with the data files from DBSR complex. All utility program provide short instructions by question mark **?** as first argument in the command line.

Quick-references to the utilities

dbound_tab	produces the total list of resulting bound states after DBSR calculations
dbound_bsw	converts the close-coupling B-spline expansions to the c- and bsw-files for individual state
dbsw123	merging the set of bsw-files with user's choice of orbitals and with optional changing the spectroscopic notation
rw123	merging the set of GRASP w-files with choice of orbitals and with optional changing the spectroscopic notation
rw_bsw	converts the GRASP w-file to DBSR bsw-file
bsw_rw	converts the DBSR bsw-file toGRASP w-file
dbsr_merge	merging a set of (name.c, name.bsw) files to one pair (merge.c, merge.bsw) with consistent set-indexes if orbitals are not-orthogonal
rw_tab	prepares the text files (one for each orbital) suitable for plotting the radial functions from w-file
bsw_tab	prepares the text files (one for each orbital) suitable for plotting the radial functions from bsw-file

D B O U N D _ T A B

Description:	produces the total list of resulting bound states
Input files:	**dbound.nnn**
Output files:	**dbound_tab**
Call as:	**dbound_tab** [optional arguments]

This program sorts the energies of states recorded in different **dbound.nnn** files and prints them in atomic units, eV or cm^{-1}, relative to the lowest state. The user can define the range of partial waves and the energy range to restrict the output. The end of the file contains the parameters used by program. The range of partial waves is defined by **klsp1**, **klsp2**, and **klsp3**, as the initial, final and step for partial wave. **Emin**, **Emax** restrict the energy region under consideration (zero values mean no restrictions). Nuclear charge **Z** and **AWT** (if they are not zero) are used to define conversation factor from atomic units (Ry, au) to other units (eV, cm-1). **E0** defines the reference points to calculate excitation or bound energies. If reference point is not defined by user, the program chooses the energy of the first target state as the reference points. All above parameters can be redefined by corresponding command-line arguments (as parameter=value), or user can change these parameters directly in the **dbound_tab** file and re-run the program.

```
klsp state  label            2J  π    E(Ry)     E(eV)    E(cm-1)       E(au)
   1  1   4p-2.4p4.5s.1/2     1  1  -0.15279  -4.15757  -33533.1  -2979.81868102
   2  1   4p-2.4p4.5p-.1/2*   1 -1  -0.09596  -2.61106  -21059.6  -2979.76184733
   3  1   4p-2.4p4.5p.3/2*    3 -1  -0.09480  -2.57961  -20805.9  -2979.76069159
   5  1   4p-2.4p4.4d.5/2     5  1  -0.06517  -1.77337  -14303.2  -2979.73106279
   4  2   4p-2.4p4.4d-.3/2    3  1  -0.06506  -1.77037  -14279.0  -2979.73095257
   1  2   4p-2.4p4.6s.1/2     1  1  -0.06140  -1.67078  -13475.7  -2979.72729237
   2  2   4p-2.4p4.6p-.1/2*   1 -1  -0.04533  -1.23344   -9948.4  -2979.71122058
   3  2   4p-2.4p4.6p.3/2*    3 -1  -0.04496  -1.22341   -9867.5  -2979.71085200
.....................................................................................
  11 20   4p-2.4p4.kh.11/2*  11 -1   0.32611   8.87392   71573.0  -2979.33977945
  10 20   4p-2.4p4.kh-.9/2*   9 -1   0.32611   8.87392   71573.0  -2979.33977943
*

Z    =  37.000
AWT  =   0.000

E0   =     -2979.66589212
Emin =    -37557.73046045
Emax =         0.00000000

klsp1 =   1
klsp2 =  99
klsp3 =   1

au_eV=        27.211214
au_cm=    219473.263205
cm_ev=      8065.544781

nstate =  218
```

Figure 1. Example of the **dbound_tab** file.

D B O U N D _ B S W

Description:	converts the close-coupling *B*-spline expansions to the *c*- and *bsw*-files for individual state
Input files:	**dbound.nnn, dbound_bsw.inp** (optional)
Output files:	*c*- and *bsw*-files for indicated states, **name.c** and **name.bsw**
Call as:	**dbound_bsw mode=** (if given input file **dbound_bsw.inp**), or **dbound_bsw klsp=... state=... name=...** , where **klsp** - partial wave index **state** - state index' **name** - name for given state

The results of the bound-state *B*-spline calculations are recorded in the **dbound.nnn** files in the form of the corresponding close-coupling expansions (7.3). The DBOUND_BSW utility collects the information for the bound states indicated in the file **bound_bsw.inp**, and records it as pair **name.c** and **name.bsw**. These files can be used as input target states files for other DBSR calculations, or for calculations different atomic parameters, such as oscillator strengths, etc.

Input file is usually created on the base of the **dbound_tab** file created by utility DBOUND_TAB and contains the list of states to be processed. Example is given in Fig.13.5. Each line contains the information for one state as index of the partial wave, index of the state for given partial wave and assigned name. Asterisk denotes the end of the list. The names are usually assigned by user. In case of large-scale calculations with hundreds of states, it is more convenient to use additional optional argument **mode**. In this case, all names are assigned automatically as **mode_nnn_mmm**, where **nnn** – index of partial wave, **mmm** – index of state. If needed to output a few individual states, the user can employ the command-argument option indicated above.

Figure 2. Example of the **dbound_bsw.inp** file obtained on base of the information in the **dbound_tab** file, Fig. 1.

```
     1     1    5s1
     2     1    5p1
     3     1    5p3
     5     1    4d5
     4     2    4d3
*
```

DB S W 1 2 3

Description:	merging the set of bsw-files with user's choice of orbitals and with optional changing the spectroscopic notation
Input files:	set of bsw-files under consideration
Output files:	resulting **bsw-file** with chosen orbitals
Call as:	**dbsw123 +** interactive input (knot.dat is not required)

R W 1 2 3

Description:	merging the set of GRASP w-files with choice of orbitals and with optional changing the spectroscopic notation
Input files:	set of w-files under consideration
Output files:	resulting **w-file** with chosen orbitals
Call as:	**rw123 +** interactive input

R W _ B S W

Description:	convert the GRASP w-file to DBSR bsw-file
Input files:	**name.w + knot.dat**
Output files:	**name.bsw**
Call as:	**rw_bsw name.w**

B S W _ R W

Description:	convert the double (p,q) B-spline representation of one-electron orbitals, *bsw*-files, to the GRASP package format, *w*-files
Input files:	**name.bsw**
Output files:	**name.w**
Call as:	**rw_bsw name.w**

D B S R _ M E R G E

Description:	merging a set of (name.c, name.bsw) files to one pair (merge.c, merge.bsw) with consistent set-indexes if orbitals are not-orthogonal
Input files:	set of c- and bsw-files
Output files:	**merge.c + merge.bsw** or given by parameter out
Call as:	**dbsr_merge F1.c F2.c ...** [key-words parameters] **dbsr_merge inp=...** [key-word parameters]
	key-words parameters (optional): **out** [merge] - name for resulting c- and bsw- files .c **jjmin** [-1] - minimum 2J value (-1 means no optional) **jjmax** [-1] - maximum 2J value (-1 means no optional) **eps_ovl** [1.d-7] - tolerance for one-electron overlaps (optional) **eps_core** [1.d-5] - tolerance for overlaps with core functions (optional) **inp** - input file if any

List of merging c-files are defined as not key-words arguments. This list (F1.c, F.2.c, ...), along with other parameters, can also be given in input file defined through **inp**=..., with one filename per line. The order of parameters or merging file does not matter.

RW_TAB

Description:	prepares the text files (one for each orbital) suitable for plotting the radial functions from w-file
Input files:	**name.w**
Output files:	**name.nl1, name.nl1, name.nl1, ...**
Call as:	**rw_dat name.w**

DBSW_TAB ???

Description:	prepares the text files (one for each orbital) suitable for plotting the radial functions from bsw-file
Input files:	**name.bsw**
Output files:	**name.nl1, name.nl1, name.nl1, ...**
Call as:	**dbsw_tab name.bsw**