## 20. Program BSR_BMAT (version 4)

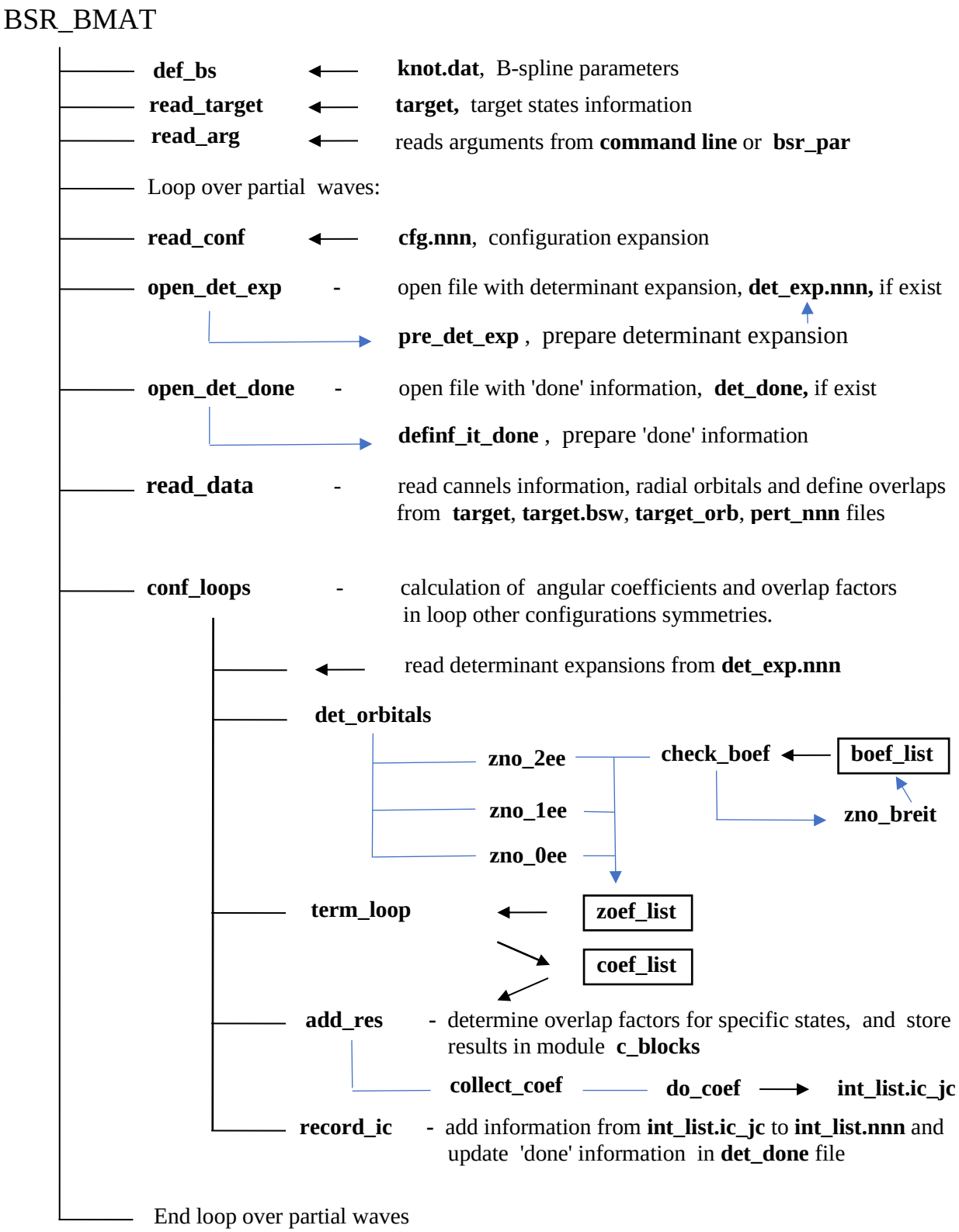
### *20.1. Outline of the BSR_BMAT calculations*

The BSR_BMAT program is designed for the large-scale calculations and is the combination of the BSR_BREIT and, partly, BSR_MAT programs. Its goal is to create the list of the angular coefficients for the specific configuration expansion. It means that the results can be applied only to the given configuration expansion with the specific one-electron orbitals, whereas the angular-coefficient datasets after BSR_BREIT can be applied to variety of configuration expansions with different one-electron orbitals. These general datasets may require very big memory in case of the large-scale calculations with configurations with several open shells (e.g., open 3d-shells for iron-group elements). Large memory requirements are due to huge amount for overlap factors in this case. BSR_BMAT computes all overlaps factors, so the resulting dataset contains only the list of the one- and two-electron integrals and the corresponding numerical coefficient.

The logical structure of BSR_BMAT the same as in the BSR_BREIT program. The only difference that in the last step, after the calculations of angular coefficients, the BSR_BMAT program estimates the all overlap factors for the given configuration expansion.

The BSR_BMAT program has the time-interrupt option, governed by the **time** parameter. If program did not complete all computations for the given time, it stops and record additionally the interrupt point in the file **det_done.nnn**. The determinant expansions are also recorded in the **det_expn.nnn** file. It prevents the lost of data in case than the ordered time is not enough for full calculations and allows one to continue computations in the repeated calculations.

The final results are recoded in the file **int_list.nnn**. The program BSR_MAT4 switches to these data by parameter **mode_bp**=1.




**F**ig. 7.1. Block diagram for the program BSR_BMAT and data flow.

*20.2. Data files*

The BSR_BMAT uses all the files indicated in the description of the BSR_BREIT and BSR_MAT programs. The difference is in the final results files specified below.

| | |
|---|---|
| **int_list.nnn** | File type: unformatted sequential output.<br>Created by program BSR_BMAT, routine **do_coef**.<br>Read by routine **state_res_bp** in BSR_MAT4 program.<br>Description: databank for angular coefficients for specific ACS. |
| **det_expn.nnn** | File type: unformatted sequential output.<br>Created by routine **pre_det_expn**.<br>Read by program BSR_BMAT for repeating calculations.<br>Description: determinant expansions for given ACS. |
| **det_done.nnn** | File type: unformatted sequential output.<br>Created by routine **record_it_done**.<br>Read by program BSR_BMAT for repeating calculations.<br>Description: indicate the angular symmetries, already processed. |

*20.2.1. Format of **int_list** file*

The angular coefficients are recorded in blocks for the specific pair of the configuration symmetries. Block structure allows to reduce the time for the read/write operations. Each block contains the following information:

1. `icase,kpol,itype,ncdatap`
   `icase` – block index
   `kpol` – multipole index
   `itype` – integral type
   `ncdata` – number of coefficient in the block

2. `(cdata(i),i=1,ncdata)` – Numerical angular coefficients with overlap estimations.

3. `(k1(i),i=1,ncdata)` – Integral indexes
4. `(k2(i),i=1,ncdata)`
5. `(k3(i),i=1,ncdata)`
6. `(k4(i),i=1,ncdata)`

*20.2.2. Format of **det_expn** file*

The determinant expansions are recoded in blocks

1. `ic,kt,kdt,Ltotal,Stotal,MLT,MSTi`
   `ic` – block index
   `kt` – number of terms
   `kdt` – number of determinants

`Ltotal` – total orbital momentum (2L+1 value)
`Stotal` – total spin (2S+1 value)
`MLT` – magnetic orbital value ($2M_L$+1 value)
`MST` – magnetic spin value ($2M_S$+1 value)

2. `IP_kt(1:kt)` – term indexes according to **conf_LS** module.

3. `CC_det(1:kt,1:kdt)` – expansion coefficients.

4. `IM_det(1:ne,1:kdt)` – one-electron orbitals *ml*-values, `ne` – number of electrons.

5. `IS_det(1:ne,1:kdt)` – one-electron orbitals *ms*-values, `ne` – number of electrons.

6. `Nsym(1:ne)` – subshell indexes

7. `Lsym(1:ne)` – orbital momentum value

The above block are repeated for all involved cases. In the and of file we have record with the number of the cases:

8. ic_case

*20.2.3. Format of **det_done** file*

1. `ic_case` – number of cases
2. `IS_NEED (1: ic_case*(ic_case+1)/2)`

IS_NEED = 0 – means that the corresponding case are not processed yet.