The preparation of the trace.txt file with the "vasp2trace" code

1. Download and install the "vasp2trace" source code.
   - tar -zxvf src_trace_v1.tar.gz
   - cd src_trace_v1
   - make
2. Run the VASP code (*e.g.,* vasp.5.3.3) to obtain the wavefunctions (WAVECAR) at the high-symmetry k-points (KPOINTS). The list of high-symmetry k-points for each space group is given in the folder "max_KPOINTS_VASP".
   - Run a self-consistent calculation with "ISTART = 0 ; ICHARG = 2".
   - Run a band-structure calculation with "ICHARG = 11 ; LWAVE= .True. (default)".
   - Run src_trace_v1/vasp2trace in the folder.
     – Only OUTCAR and WAVECAR files are used to obtain the symmetry operators and coefficients of the plane waves, respectively. "trace.txt" is generated as the result of the computed traces for degenerate bands (with an energy tolerance of 0.002 eV).
     CAUTIONS: The list of coordinates KPOINTS in the file "max_KPOINTS_VASP" are given in a primitive basis of the reciprocal space. The transformation from the standard setting of the space group to the chosen privitive basis in direct space is defined in the following section.
3. Upload the file "trace.txt" on the BCS.

The transformation from the standard setting to the primitive unit cell chosen

There are only seven different types of lattices, *i.e.* P, C, B, A, R, F and I. In the X type, the primitive lattices ($\vec{p}_1$, $\vec{p}_2$, $\vec{p}_3$) are defined by a transformation matrix M_X.

$$\left(\vec{p}_1 \;\; \vec{p}_2 \;\; \vec{p}_3 \right) = \left(\vec{c}_1 \;\; \vec{c}_2 \;\; \vec{c}_3 \right) \cdot M_X$$

where $\vec{c}_1$, $\vec{c}_2$ and $\vec{c}_3$ form a basis of the lattice in the standard (or default) setting. All the matrices M_X are given as follows:

$$M_P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad M_C = \begin{pmatrix} 0.5 & 0.5 & 0 \\ -0.5 & 0.5 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$M_B = \begin{pmatrix} 0.5 & 0 & -0.5 \\ 0 & 1 & 0 \\ 0.5 & 0 & 0.5 \end{pmatrix} \qquad M_A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0.5 & -0.5 \\ 0 & 0.5 & 0.5 \end{pmatrix}$$

$$M_R = \begin{pmatrix} 2/3 & -1/3 & -1/3 \\ 1/3 & 1/3 & -2/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix} \qquad M_F = \begin{pmatrix} 0 & 0.5 & 0.5 \\ 0.5 & 0 & 0.5 \\ 0.5 & 0.5 & 0 \end{pmatrix}$$

$$M_I = \begin{pmatrix} -0.5 & 0.5 & 0.5 \\ 0.5 & -0.5 & 0.5 \\ 0.5 & 0.5 & -0.5 \end{pmatrix}$$

If you have any problem using this program and/or any question or suggestion, please contact its author, Zhijun Wang, at the address: zjwang.phy@mail.com