

A) Help to start a biphasic calculation:

In order to use this kind of calculation, you need to construct 2 simulated volumes. Be careful that these volumes must have exactly the same physical dimensions (in microns). You need to define manually the size of the multipole domains, and the 2 phases need to have exactly the same number of domains with the same repartition.

These volumes must have a part empty of dislocation and a part containing some dislocations, such as the empty part of the phase 1 exactly correspond to the full part of the phase 2 and reciprocally. This two part are divided with a boundary.

B)Methodology to build the 2 simulation boxes:

B-1) Build the 2 control files. The files must be the same except for the solicitation axis direction which could be different if rotation is applied on one or the both phases.

B-2) If you need rotations, build the 2 `matrice_rotation_BVD` files. Be careful that the X and Y axis of the 2 grains are inversed each other (the axis X of the phase 1 is on inverse direction that the one in the phase 2, and similarly for the axis Y).

If you don't need rotation, just write the matrix $\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ in the `matrice_rotation_BVD` file of the phase 1 (left phase)

(BE CAREFUL: with this matrix you will have the two phases separated with a boundary oriented in the (100) direction. For another kind of boundary, please calculate the adapted matrix)

B-3) Calculate the Lower Common Multiple of the 2 phases box factor.

B-4) Generate 2 segment configurations thanks to the `inputconfinet` file, with the LCM calculated previously as the box factor. Please decrease the echelle factor if this box factor is too high to generate configurations.

B-5) Adjust the dimensions of the 2 volumes such as they correspond exactly to the same physical dimensions (i.e. $\text{dim phase1} / \text{homothetie1} / \text{homothetie2} = \text{dim phase2}$)

B-6) Multiply the X dimension (if you have a boundary (100)) of the volume by 2 (in order to have a full and an empty part). Adapt the equations of the boundary and free surface in the 2 `b_plan` files

B-7) Shift the coordinates of the segments of the phase 2 such as they are in the second part of the simulated volume.

C) Modifications introduced for the bi-phase calculation:

The modification involved the 2 kinds of stress interaction calculation: the long-range interactions and the short-range ones

In the following, the main modifications introduced in these 2 parts are described.

For the calculation of long-range interactions (interactions calculated on the center of each multipole):

The main modification is the creation of two communicators (one for each phase). The global communicator `MPI_COMM_WORLD`, which is linked to all the processes involved in the microMega calculation, is split between these 2 communicators called `COMM_PAIR_IMPAIR`. The belonging of each process is described thanks to the variable `"Ma_couleur"`. So the first communicator `COMM_PAIR_IMPAIR` involves all the processes with `Ma_couleur=0`, and the second communicator `COMM_PAIR_IMPAIR` involves all the processes with `Ma_couleur=1`.

The rank of each process in `COMM_PAIR_IMPAIR` is reattributed thanks to the variable `"mon_rang_pairimpair"`.

It is important to notice that in spite of the process being a splitter between the two communicators `COMM_PAIR_IMPAIR`, the global communicator `MPI_COMM_WORLD` still exists and belongs to all the processes.

A key is created on the material file. This key is named `"Nb_phase"`.

If `Nb_phase=2`, a second set of material constants must be defined after the first set in the material file. The two sets of data are differentiated thanks to the variable `"Index_phase"`

The input files control and segment are written twice (i.e. two files exist, as example control for phase 1 and control2 for phase 1). If they are used, some other input file must be written twice too (ex: `matrice_rotation_BVD`, `b_plan`,...)

The output files will be written twice, with the title `xxxx2` for the file corresponding to the 2nd phase.

Most of the communications previously done on `MPI_COMM_WORLD` in the file `10dynam.F90` are now done on `COMM_PAIR_IMPAIR` (these calculations are only made between the processes related to the same phase).

Similarly the speed calculation related to the long range interaction calculation is made on `COMM_PAIR_IMPAIR`

One virtual segment is artificially added on each empty box when the cost calculation for each proc is made. The aim is to force the processes to use equally the empty boxes (it is necessary because we will use all the boxes of the volume when the contributions of the two phases will be added).

The long_range interactions calculated on each multipole in the 2 different phase are added thanks to an operation `MPI_ALLREDUCE` on `MPI_COMM_WORLD`

Similarly, the plastic strain calculated on the two phases are added in order to have a control on the imposed strain rate coherent for the two phase. It is important to notice that this summation on plastic strain is only used for the control, the 2 phases still remain a different strain each other.

For the calculation of the short-range interactions (only calculated between segments belonging to two neighbor multipoles)

In the file `11topolo.F90`, the equation of the boundary between the two phases is calculated, and the boxes close to this boundary are identified (first neighbor). As all part of the biphasic calculation are parallelized, the file `11topolo` is parallelized.

In the file `09elasti.F90`:

The segments contained on the boxes close to the boundary are identified and listed in the subroutine `REGION`. The box index and the centers of these segments are stored in the list `liste_RO_temp`

In the subroutine `SIGMA_INT_CP`: the parallelization parameters used for the calculation of the short-range interactions (`BDEB`,...) are used on one phase only (i.e. on `COMM_PAIR_IMPAIR`)

A second step of calculation is introduced after this classical short-range calculation. This second step is related to the segments contained in `liste_RO_temp`.

The segment center coordinates are divided by the homothetic factor linked to the slip plane orientation (if defined in `matrice_rotation_BVD`). The aim is to place these coordinate on the "standard" frame (i.e. without rotation and homothetic).

The number of segments and their center coordinates without homothetic are transmitted to the other phase (transmission on `COMM_WORLD`)

The center coordinates received (i.e. corresponding to the other phase) are multiplied by the homothetic factor

Then the calculation of the interactions across the boundary is made:

First the working domain on the box close to the boundary is defined for each process (i.e. an index of starting box and ending box is defined)

Then the short-range calculation loop is made on the segment center coordinates received

This short-range interaction is stored for all the involved segments in the list `SIG_JOINT`

The value of `SIGJOINT` calculated by each process are transmitted to the other process of the phase (on `COMM_PAIR_IMPAIR`)

The list `SIGJOINT` is transmitted to the other phase (transmission on `COMM_WORLD`). Thus the processes in charge of the phase P are now in possession of the stress value `SIGJOINT` on the center of the segments of P close to the boundary and due to the other phase.

The values of `SIGJOINT` are stored in a table `SIGMA_JOINT` defined for all segments (`=0` for the segments far from the boundary). This table `SIGMA_JOINT` is added to the total stress contribution on each segment.