Usage of the convert_CMconfigs program, converting RMC configuration to CrystalMaker *.cmtx file

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Both the text type and the binary configurations file of RMC_POT can be converted to the text type *.*cmtx* file of the visualization software CrystalMaker. The converter is self-explanatory, and needs a parameter file to contain the conversion details.

It can use the **.cfg*, **.bcf* or **_coll.cfg* file for RMC coordinate file input, the last one being the text type configuration file produced with RMC with collecting the configurations options containing multiple configurations consecutively.

It is possible to convert only a part of the configurations, if nopt all the atoms required for the visualization, this is governed by the mode option, there are 4 possible ways to select the atoms.

- option 1: The indices of the specified number of atoms for each type will be spread among the atoms of this type with as equal step as possible. As usually atoms with similar indices are close to each other, especially if no swaps were used during the simulation, this way the atoms can be found everywhere in the simulation box.
- option 2: The first given number of atoms will be used from a type. (Most probably atoms close to each other are chosen this way!)
- option 3: Atoms of given indices specified at the end the parameter file will be selected. (Index can range from 1 -> ntotal, and has to follow the order of atom types.)
- option 4: Only particles between two parallel planes will be saved into the file. The planes have to be parallel to one of the sides of the simulation box! There have to be an integer after option 4 to specify which axis is perpendicular to the cutting plane (x:0, y:1, z:2), followed by two real numbers between -1 and +1) to specify the reduced coordinates, between which the atoms will be outputted. Example for this line of the parameter file choosing the atoms, with reduced y-coordinates are between -0.7 -> 0.5: 4 1 -0.7 0.5.

If all the atoms of a configurations has to be selected, then the quickest way to do it to use option 2 and give the number of all the atoms of each type to use.

An example parameter file is given here:

```
ccl4.cfg          ! name of the input configuration file
5                 ! number of configurations to convert (only meaningful for *coll.cfg)
2                 ! number of used types
3 1 –0.7 0.5      ! mode option (for option 4 index of the perpendicular axis(x:0, y:1,z:2),min, max reduced coord)
C  2              ! Atom's chemical symbol, number of atoms to use for each type
Cl 8              ! Atom's chemical symbol, number of atoms to use for each type
1                 ! Atom indices to select, only in case of option 3
2                 ! Atom indices to select, only in case of option 3
2049              ! Atom indices to select, only in case of option 3
4097              ! Atom indices to select, only in case of option 3
6145              ! Atom indices to select, only in case of option 3
8193              ! Atom indices to select, only in case of option 3
2050              ! Atom indices to select, only in case of option 3
4098              ! Atom indices to select, only in case of option 3
6146              ! Atom indices to select, only in case of option 3
8194              ! Atom indices to select, only in case of option 3
```

The green part has to be included only for option 4, the blue for option 3, the number of atoms denoted by pink only for options 1-3.

If no atoms of an atom type ha to be used in case of option 1-3, than give zero for the number of atoms.

The name of the output file will be generated by the input file by replacing the original file extension by *.*cmtx*. The program will decide based on the original file extension about the type of the input file, so it is important, that the original RMC file extensions should be used, (*.*cfg* 1 text type configuration, *.*bcf* 1 binary configuration, *_*coll.cfg* multiple text configurations. In case of multiple configurations atoms of the first *nconfig* configuration will be selected for output, and put into separate files with name *_*coll000X.cmtx*.

The program can be started by **executablename** then it asks for the parameter file name, or by **executablename parfilename**