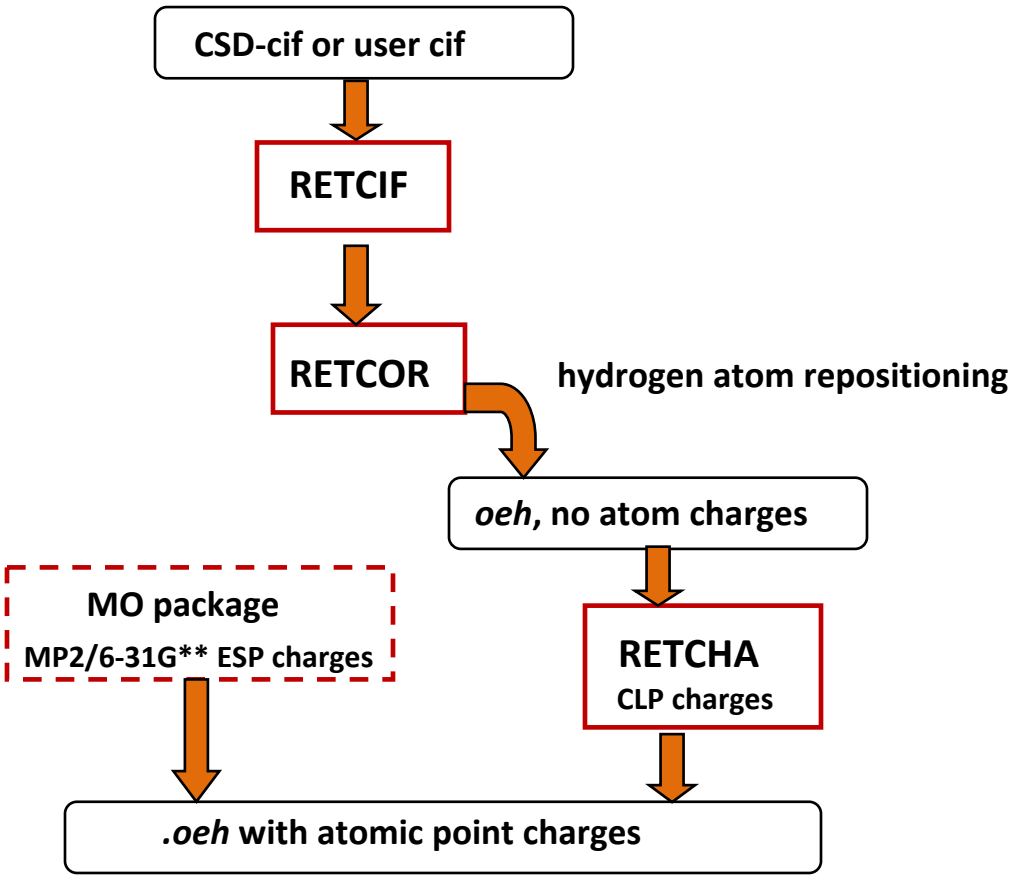
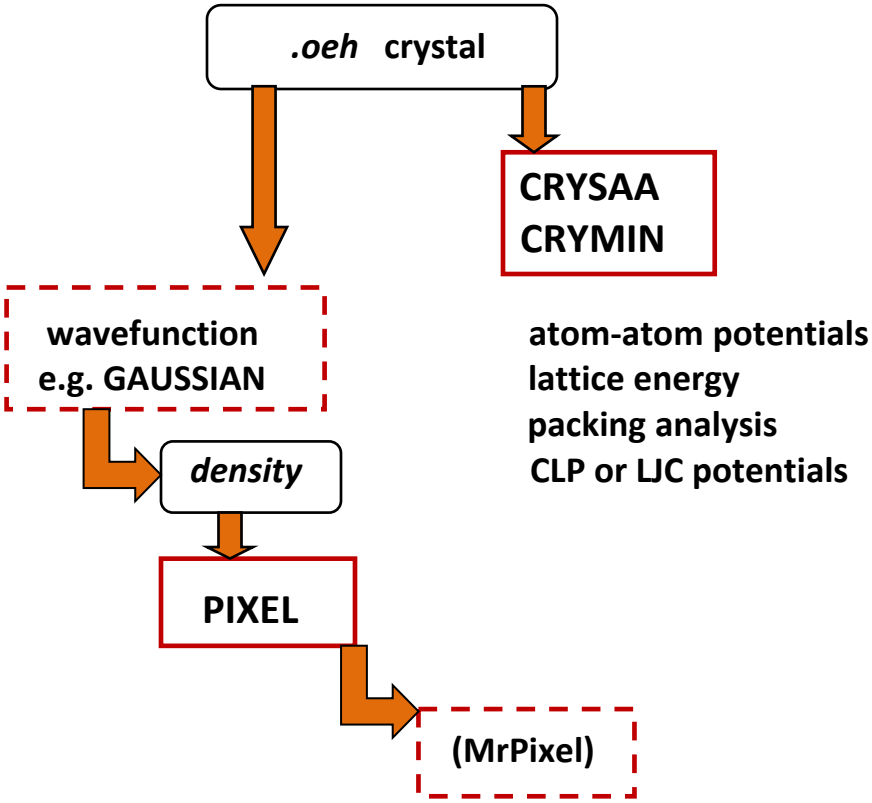
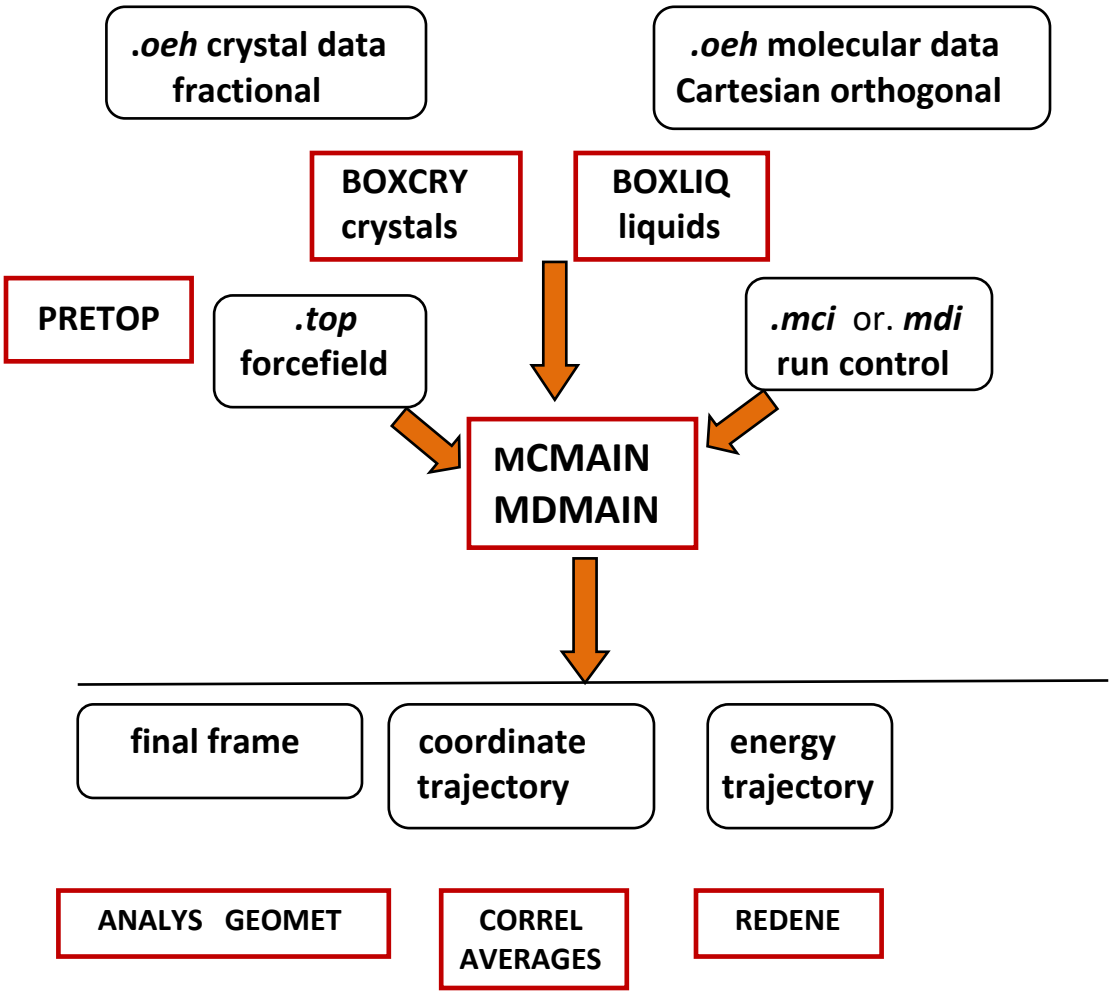


Flowchart of the data retrieval, hydrogen positioning and point charge calculations. The MO package does not belong in MiCMoS. The .oeh file is the main format for molecular geometric information

Throughout this document: Red squares: program modules; blue rings: files.



Flowchart of the atom-atom and PIXEL lattice energy calculation modules. A PIXEL version (MrPixel) linking to post-analysis scripts can be downloaded from crystal.chem.ed.ac.uk/software/coulomb-london-pauli-clp-pixel under local control at University of Edinburgh.
Dotted modules are external to MiCMoS.



Flowchart of the Monte Carlo and Molecular Dynamics modules, with their satellites for force field generation, computational box preparation, trajectory analysis. Many more modules perform other tasks such as preparation of solutions, of embedded clusters, geometry checks of various kind.