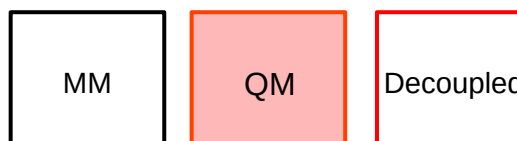
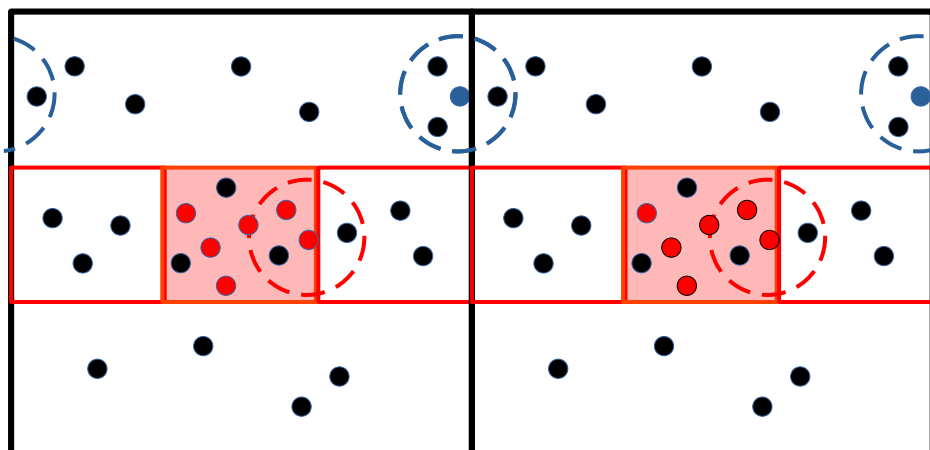


● QM atom ● MM atom ○ Real-space cutoff

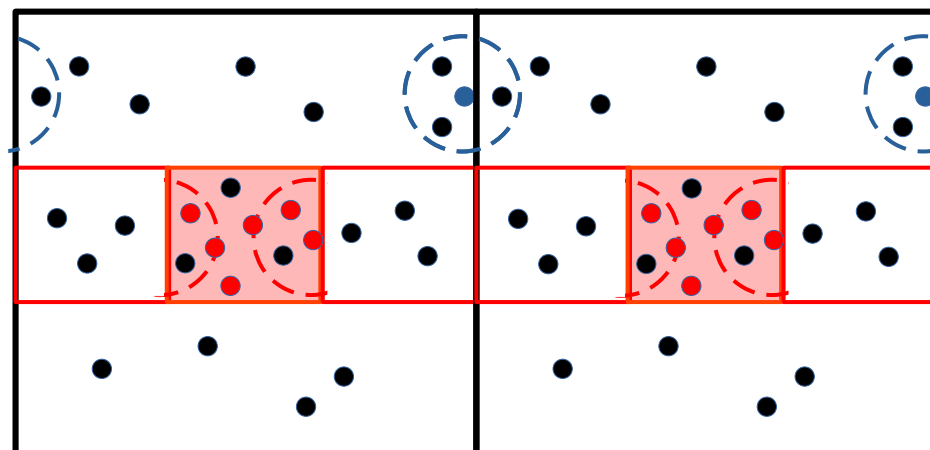


1) CELL SUBSYS XYZ QMMM NONE
POISSON DFT XYZ MM XYZ QMMM XYZ



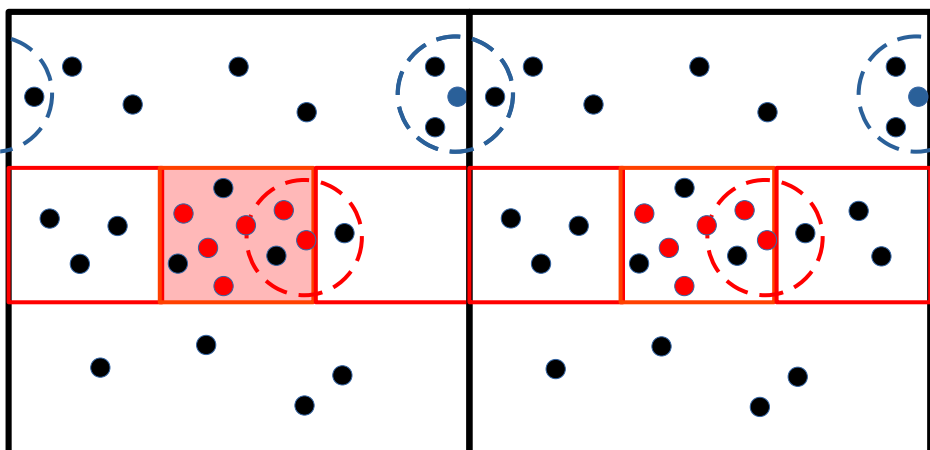
QM part interacts with QM and MM periodic images.
Decoupling of QM images is achieved with the Blöchl technique.
Pair lists for the QM atoms are built taking into account the periodicity of the MM box.

2) CELL SUBSYS XYZ QMMM XYZ
POISSON DFT XYZ MM XYZ QMMM XYZ



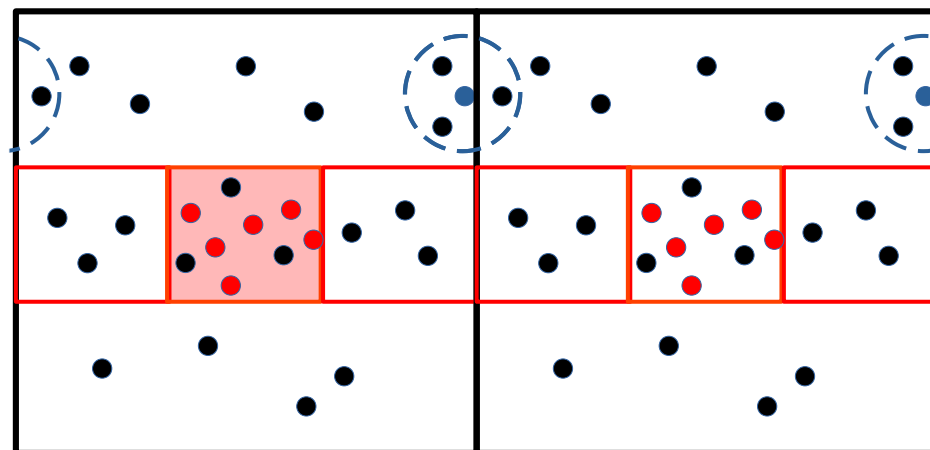
QM part interacts with QM and MM periodic images.
Decoupling of QM images is achieved with the Blöchl technique.
Pair lists for the QM atoms are built taking into account the periodicity of the QM box.

3) CELL SUBSYS XYZ QMMM NONE
POISSON DFT NONE MM XYZ QMMM XYZ



QM part only interacts with MM periodic images.
Decoupling is achieved with DFT Poisson solver (e.g. MT).
Pair lists for the QM atoms are built taking into account the periodicity of the MM box.

4) CELL SUBSYS XYZ QMMM NONE
POISSON DFT NONE MM XYZ QMMM NONE



QM part is isolated from all periodic images.
Decoupling is achieved with DFT Poisson solver (e.g. MT).
Pair lists for the QM atoms are not necessary.