creating supercells with cif2cell

The use of cif2cell, including how to create supercells, is eloquently described by its creator Torbjörn Björkman in the cif2cell manual. You might want to read section 4 on supercell generation. The next few paragraphs are a basic summary.

Another useful source for help is

```
cif2cell –help
```

getting prepared

Let us assume you have as starting point a cif file for a primitive cell of a bcc lattice, for instance ferrite (http://www.crystallography.net/cod/9008538.cif in COD)

```
wget http://www.crystallography.net/cod/9008538.cif
```

This is a cif file with symmetry information, describing the primitive cell of ferrite. You know that this is the way to convert it into an input file for Quantum Espresso, sticking to the primitive cell:

```
cif2cell 9008538.cif -p quantum-espresso -o ferrite-primitive.in
```

The `--no-reduce` option creates a conventional unit cell instead:

```
cif2cell 9008538.cif -p quantum-espresso -o ferrite-conventional.in
--no-reduce
```

You can inspect both cells in XcrysDen:

```
xcrysden --pw_inp ferrite-primitive.in
```

```
xcrysden --pw_inp ferrite-conventional.in
```

creating bulk supercells

So far, nothing new. Let us now create a 2x1x1 supercell of both cells (=doubling the cell along the **a** lattice vector, while keeping the **b** and **c** lattice vectors as they were). These are the commands:

```
cif2cell 9008538.cif -p quantum-espresso -o ferrite-primitive-
211reg.in --supercell=[2,1,1]
```

```
xcrysden --pw_inp ferrite-primitive-211reg.in
```

You see the doubling visually. This supercell has 2 atoms.

Everything is easier to imagine if we base ourselves on the conventional cell. This happens by adding `--no-reduce` with `--supercell`: in that case, the supercell is expressed with respect to the conventional cell:

```
cif2cell 9008538.cif -p quantum-espresso -o ferrite-conventional-211reg.in --supercell=[2,1,1] --no-reduce
```

```
xcrysden --pw_inp ferrite-conventional-211reg.in
```

You can count visually that this is a supercell with 4 atoms, which is reflected in the 4 coordinate lines that are in the *.in file.

There is a more explicit way to define the same supercell: specifying three lattice vectors for the supercell (where it is the responsibility of the user to make sure that these are commensurate with the underlying lattice). Let us do this for the conventional cell:

```
cif2cell 9008538.cif -p quantum-espresso -o ferrite-conventional-211vec.in --supercell=[[2,0,0],[0,1,0],[0,0,1]] --no-reduce
```

```
xcrysden --pw_inp ferrite-conventional-211vec.in
```

You'll see the same cell with 4 atoms you found before. The power of this explicit command becomes obvious once you start creating supercells that are oriented differently with respect to the original cell. For instance:

```
cif2cell 9008538.cif -p quantum-espresso -o ferrite-conventional-rotatedvec.in --supercell=[[2,2,0],[-2,2,0],[0,0,1]] --no-reduce
```

```
xcrysden --pw_inp ferrite-conventional-rotatedvec.in
```

This is a supercell with 16 atoms, that is not a simple stacking of conventional cubes.

Creating supercells this way, would be useful to calculate and visualize charge density differences in planes that are not parallel to the faces of the unit cell. Say, for instance, the (1,1,0) plane of the conventional ferrite cell. You could make this supercell, in which the (1,0,0) face of the supercell is the (1,1,0) plane of the original cell:

```
cif2cell 9008538.cif -p quantum-espresso -o ferrite-conventional-110.in --supercell=[[1,1,0],[-1,1,0],[0,0,1]] --no-reduce
```

```
xcrysden --pw_inp ferrite-conventional-110.in
```

point defects in crystals

Another reason to use supercells, is to mimic an impurity in a host lattice. Create a 2x2x2 supercell of ferrite, and replace one Fe-atom by a Cu atom:

```
cif2cell 9008538.cif -p quantum-espresso -o ferrite-conventional-222reg.in --supercell=[2,2,2] --no-reduce
```

```
nano ferrite-conventional-222reg.in
```

Tell in the &SYSTEM block that there are 2 different elements now:

```
&SYSTEM
  ibrav = 0
  A =    2.94000
  nat = 16
  ntyp = 2
/
```

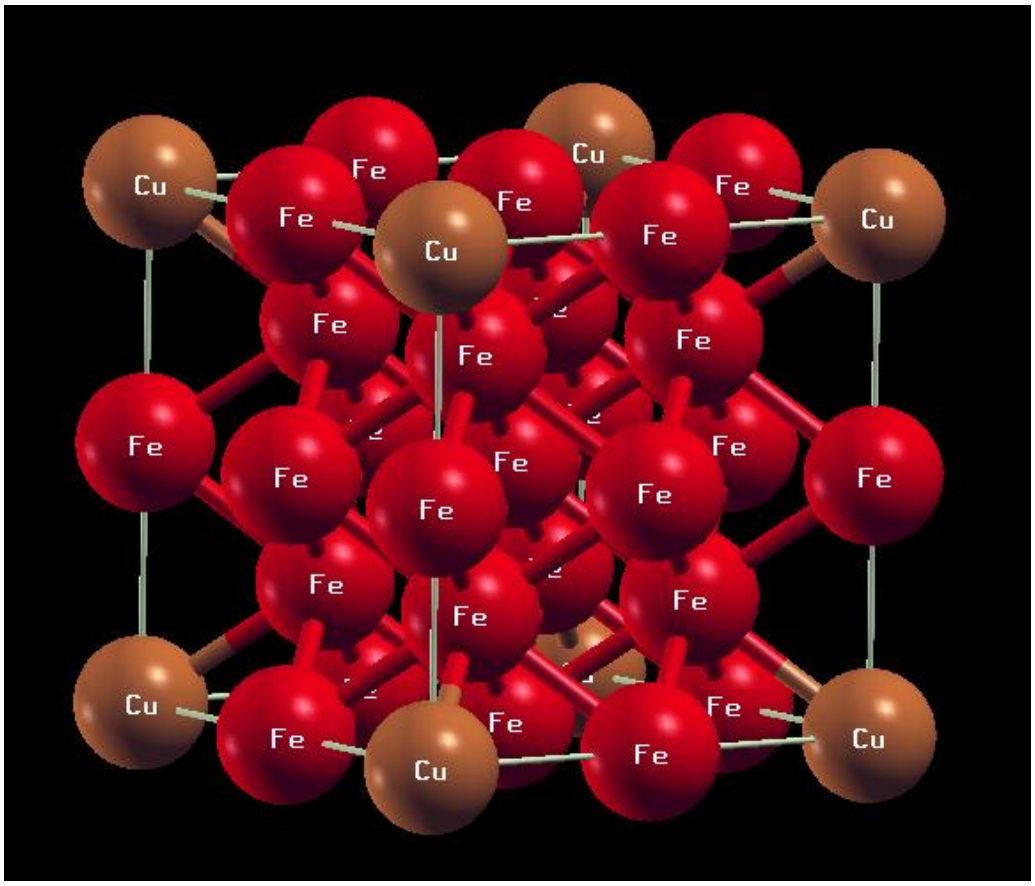
Change one of the position lines to Cu, and add a line for the Cu pseudopotential of your choice:

```
ATOMIC_SPECIES
  Fe    55.84500  Fe_PSEUDO
  Cu    63.54600  Cu_PSEUDO

ATOMIC_POSITIONS {crystal}
Cu    0.000000000000000   0.000000000000000   0.000000000000000
Fe    0.250000000000000   0.250000000000000   0.250000000000000
Fe    0.500000000000000   0.500000000000000   0.000000000000000
```

Call this modified cell ferrite-conventional-222regCu.in, and visualize it:

```
xcrysden --pw_inp ferrite-conventional-222regCu.in
```



If you want to feel how this really mimics an 'isolated' substitutional impurity in a lattice, let xcrysden display a larger part of the crystal (Modify/Number of units drawn/ 4 x 4 x 4 / Update / OK).

You can isolate the impurity more, by doing the same single replacement in a 3x3x3 cell, or in a 4x4x4 cell,… Obviously, the subsequent DFT calculations will rapidly become more expensive.

A small exercise:

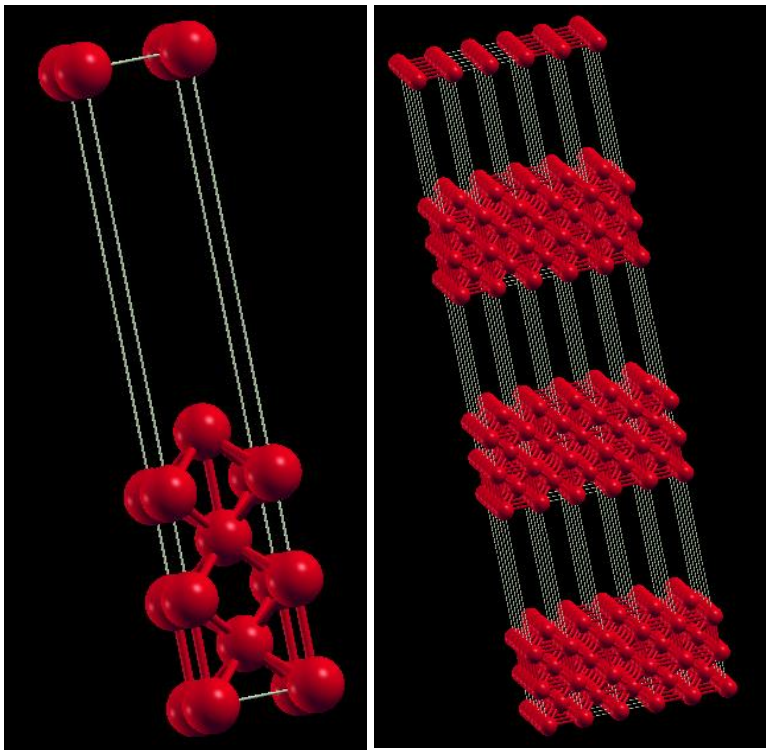
- How would you make a supercell for a carbon atom that is an octahedral interstitial impurity in ferrite?
- How would you make a supercell for a single atom vacancy in ferrite?

supercells for surfaces

A third reason to make supercells, is to create surfaces. Let us insert a vacuum layer with a width equal to three unit cells to create a (001) surface in ferrite:

```
cif2cell 9008538.cif -p quantum-espresso -o ferrite-001-surface.in --supercell=[1,1,3] --no-reduce --supercell-vacuum=[0,0,1]
```

In this example, 3 conventional unit cells are stacked on top of each other, followed by the same amount of vacuum (the amount of vacuum is measured in terms of the lattice vectors of the supercell without vacuum – hence 3=1). Visually:



Creating a (110) surface would happen this way:

```
cif2cell 9008538.cif -p quantum-espresso -o ferrite-110-surface.in --supercell=[[3,3,0],[-3,3,0],[0,0,3]] --no-reduce --supercell-vacuum=[0,1,0]

xcrysden --pw_inp ferrite-110-surface.in
```

some exercises :

- Play with the previous command, until you understand why the supercell+vacuum which you get look the way they do.
- Convince yourself that the positions of the atoms in a (001) surface is different from the positions in a (110) surface.
- Create a supercell with a (110) surface where
    - One of the surface atoms is replaced by another element
    - An impurity atom is added on top of the surface

supercells for free atoms

Another use of a supercell is to mimic free atoms with a periodic DFT code. In principle, the distance between the single atom in the supercell and its periodic images should be so large that any interaction between them is zero. In reality, some spurious background interaction is unavoidable (unless you would make the lattice parameter of the supercell extremely large, which would make the calculation very time-consuming: vacuum requires as many plane waves in the basis set as space filled by atoms does). In order to make this spurious background interaction as innocent as possible, we better make it as isotropic as possible. For that reason, a supercell with fcc symmetry is often used. In the fcc cell, the 'isolated' atom has as many as 12 distant first nearest 'neighbours', which is a better approximation to an isotropic surrounding than the alternatives of 8 neighbours (bcc) of 6 neighbours (simple cubic).

A cif file for a fcc supercell for an isolated atom is available here. You can convert it to a regular input file for Quantum Espresso in the usual way. If you run such a free atom calculation, be sure to make a spin-polarized (a.k.a. 'magnetic') calculations (see here how to do that in Quantum Espresso). Indeed, in free atoms the number of spin-up and spin-down electrons is often not identical (Hund's first rule). If you would force them to be equal by a non-magnetic calculation, then the total energy of the free atom would be higher than the ground state total energy. This would introduce an error in, for instance, cohesive energy predictions. Verify after the calculation whether the spin magnetic moment of the supercell is identical to what you expect from the free atom ground state. For DFT codes that strictly apply symmetry, it might be needed to break the cubic symmetry (e.g. by making the a, b and c lattice parameters very slightly unequal to each other).

As a final exercise, you can create a supercell for a (001)-surface of the NaCl crystal, having 7 layers in the slab and some amount of vacuum, with a Si atom on top of the surface (at a lattice position where in the infinite NaCl crystal a Na or Cl atom would be). Periodic images of the Si atom should be 4 lattice parameters away from each other. No need to do a DFT calculation for this supercell, the goal of the exercise is to create the supercell only. Report the cif2cell command you use, describe manual modifications, and show a picture from Vesta or XcrysDen.