creating supercells with VNL

In the Builder of VNL, you can create supercells by selecting in the right panel 'Bulk Tools/supercell'.

What you see there, is a matrix. It expresses the lattice vectors of the supercell in terms of the lattice vectors of the initial unit cell.

The diagonal elements are most straightforward to interpret: when the diagonal reads 2 1 1 (an all off-diagonal elements are zero), then the supercell will be a cell that is doubled in the a-direction. Click 'Transform' to see this. If you would have taken 2 2 2 on the diagonal instead, the supercell would be doubled in all three directions.

You can now export this supercell to the input format for your DFT code as usual.

Supercells of which the lattice vectors are not parallel to the lattice vectors of the initial cell, can be created by using the off-diagonal elements of the matrix. You may experiment with this (not all choices are possible), but we will not go into this.

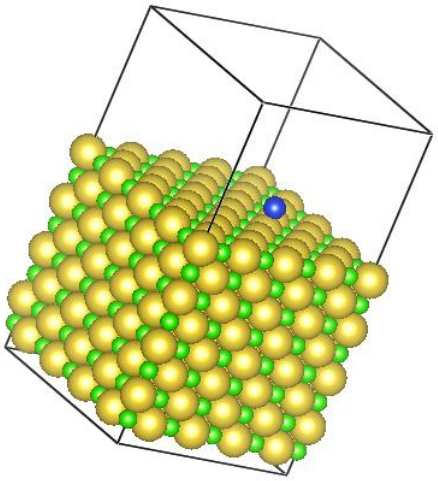
If you want to delete atoms (to create vacuum for a surface slab, for instance), you can click on an individual atom and press the delete key. The leftmost item of the top bar allows you to select a range of atoms to delete at once. If you select an atom (or a range) and click on the icon with 'Si' in the top bar, you can change the element.

Some of these changes like replacing an element or deleting atoms can also be done in the cif file or QE input file directly, as you wish.

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 an exercise, you can create a supercell for a (001)-surface of the NaCl crystal, having 7 layers in the slab and some 'layers' of vacuum, with a Si atom on the surface (at a lattice position where in the infinite NaCl crystal a Na or Cl atom would be). No need to do a DFT calculation for this supercell, the goal of the exercise is to create the supercell. (hint: if you start from a cif file that shows the primitive unit cell for NaCl with 2 atoms, you may want to use in VNL
Bulk Tools/Supercell/Conventional -> Transform
to generate the more familiar cubic unit cell with 8 atoms) After exporting and visualizing the cif file, Vesta should show a picture like the one at the right.



In case you met problems, you should describe them in the form.